rigure i

| ATOM THA | . 6 | igom Tope | Res. | | <u>x</u> | <u>Y</u> | <u>Z</u> | OCC B | MOL |
|----------|----------|--------------|-------|---|----------------|----------|----------|------------|------|
| VI TOA | DEMARK | | | | | | | | |
| ATOM MA | 100 | С | GLY | l | 69 32 5 | 51.394 | 17.320 | 1.00 31 75 | CPS1 |
| MOTA | 4 | 0 | GLY | 1 | 69.833 | 51.813 | 16 277 | 1.00 31.77 | CPS1 |
| MOTA | 3 | N | GLY | 1 | 70.959 | 52.760 | 18.620 | 1.00 35 37 | CPS1 |
| MOTA | 4 | CA | GLY | 1 | 70.031 | 51.571 | 18.653 | 1.00 32.48 | CPS1 |
| ATOM | 5 | N | ILE | 2 | 68.153 | 50.776 | 17.347 | 1.00 28.47 | CPS1 |
| ATCM | 6 | CA | ILE | 2 | 67.404 | 50.567 | 16.121 | 1.00 26.25 | CPS1 |
| ATCM | 7 | CB | ILE | 2 | 66.717 | 49.195 | 16.134 | 1.00 25.90 | CPS1 |
| ATOM | 8 | CG2 | ILE | 2 | 65.743 | 49.071 | 14.958 | 1.00 25.20 | CPS1 |
| MOTA | 9 | CG1 | ILE | 2 | 67.788 | 48.104 | 16.055 | 1.00 28.58 | C2S1 |
| MOTA | 10 | CD1 | ILE | 2 | 67.235 | 46.714 | 16.136 | 1.00 29.70 | CPS1 |
| MOTA | 11 | C | ILE | 2 | 66.379 | 51.671 | 15.959 | 1.00 24.77 | CPS1 |
| ATOM | 12 | 0 | ILE | 2 | 65.635 | 51.988 | 16.893 | 1.00 24.24 | CPS1 |
| ATOM | 13 | N | TYR | 3 | 66.358 | 52.282 | 14.781 | 1.00 23.49 | CPS1 |
| ATOM | 14 | CA | TYR | 3 | 65.407 | 53.355 | 14.515 | 1.00 23.75 | CPS1 |
| ATOM | 15 | CB | TYR | 3 | 65.923 | 54.291 | 13.420 | 1.00 25.80 | CPS1 |
| ATOM | 16 | CG | TYR | 3 | 64.952 | 55.408 | 13.087 | 1.00 28.36 | CPS1 |
| ATOM | 17 | CD1 | TYR | 3 | 64.870 | 56.552 | 13.887 | 1.00 30.78 | CPS1 |
| MOTA | 18 | | TYR | 3 | 63.950 | 57.569 | 13.608 | 1.00 33.13 | CPS1 |
| MOTA | 19 | CD2 | TYR | 3 | 64.090 | 55.307 | 11.999 | 1.00 29.71 | CPS1 |
| MOTA | 20 | CE2 | TYR | 3 | 63.166 | 56.313 | 11.709 | 1.00 32.64 | CPS1 |
| ATOM | 21 | CZ | TYR | 3 | 63.102 | 57.444 | 12.517 | 1.00 34.23 | CPS1 |
| ATOM | 22 | OH | TYR | 3 | 62.204 | 58.454 | 12.225 | 1.00 36.12 | CPS1 |
| ATOM | 23 | C | TYR | 3 | 64.075 | 52.766 | 14.068 | 1.00 23.33 | CPS1 |
| ATOM | 24 | ŏ | TYR | 3 | 63.022 | 53.193 | 14.517 | 1.00 24.16 | CPS1 |
| ATOM | 25 | N | GLY | 4 | 64.130 | 51.792 | 13.166 | 1.00 21.11 | CPS1 |
| ATOM | 26 | CA | GLY | 4 | 62.909 | 51.182 | 12.672 | 1.00 20.13 | CPS1 |
| MOTA | 27 | C | GLY | 4 | 63.216 | 49.984 | 11.799 | 1.00 19.67 | CPS1 |
| MOTA | 28 | ō | GLY | 4 | 64.354 | 49.800 | 11.371 | 1.00 18.21 | CPS1 |
| ATOM | 29 | N | ILE | 5 | 62.211 | 49.145 | 11.562 | 1.00 18.70 | CPS1 |
| ATOM | 30 | CA | ILE | 5 | 62.402 | 47.985 | 10.704 | 1.00 17.69 | CPS1 |
| ATOM | 31 | CB | ILE | 5 | 62.470 | 46.666 | 11.510 | 1.00 18.45 | CPS1 |
| ATOM | 32 | CG2 | | 5 | 63.538 | 46.799 | 12.610 | 1.00 17.74 | CPS1 |
| ATOM | 33 | CG1 | | 5 | 61.103 | 46.329 | 12.127 | 1.00 17.47 | CPS1 |
| ATOM | 34 | | ILE | 5 | 61.097 | 44.956 | 12.830 | 1.00 18.74 | CPS1 |
| ATOM | 35 | C | ILE | 5 | 61.225 | 47.936 | 9.736 | 1.00 17.16 | CPS1 |
| ATOM | 36 | 0 | ILE | 5 | 60.170 | 48.525 | 10.001 | 1.00 16.88 | CPS1 |
| ATOM | 37 | и | GLY | 6 | 61.414 | 47.248 | 8.616 | 1.00 16.81 | CPS1 |
| ATOM | 38 | CA | GLY | 6 | 60.353 | 47.163 | 7.632 | 1.00 16.27 | CPS1 |
| ATOM | 39 | C | GLY | 6 | 60.398 | 45.846 | 6.893 | 1.00 17.21 | CPS1 |
| | 40 | 0 | GLY | 6 | 61.468 | 45.303 | 6.623 | 1.00 17.76 | CPS1 |
| ATOM | | N | LEU | 7 | 59.220 | 45.345 | 6.555 | 1.00 17.08 | CPS1 |
| ATOM | 41 42 | CA | LEU | 7 | 59.085 | 44.080 | 5.858 | 1.00 18.22 | CPS1 |
| MOTA | | | LEU | 7 | 58.631 | 43.006 | 6.857 | 1.00 18.52 | CPS1 |
| MOTA | 43 | CB | LEU | 7 | 58.266 | 41.643 | 6.270 | 1.00 18.46 | CPS1 |
| MOTA | 44 | CG | | 7 | 59.552 | 40.921 | 5.800 | 1.00 18.60 | CPS1 |
| MOTA | 45 | | LEU | 7 | 57.546 | 40.825 | 7.342 | | CPS1 |
| MOTA | 46 | | LEU | | | 44.246 | 4.780 | | CPS1 |
| . ATOM | 47 | | LEU | 7 | 58.025 | | 4.988 | | CPS1 |
| MOTA | 48 | 0 | LEU | 7 | 57.036 | 44.935 | 3.623 | | CPS1 |
| MOTA | 49 | | ASP | 8 | 58.240 | 43.632 | 2.558 | | CPS1 |
| MOTA | 50 | | ASP | 8 | 57.256 | 43.693 | 1.629 | | CPS1 |
| MOTA | 51 | | ASP | 8 | 57.514 | | | | CPS1 |
| ATOM | 52 | | ASP | 8 | 56.550 | | | | CPS1 |
| MOTA | 53 | | 1 ASP | 8 | 56.853 | | | | CPS1 |
| MOTA | 54 | | 2 ASP | 8 | 55.471 | | | | CPS1 |
| MOTA | 55 | С | ASP | 8 | 57.293 | | | | CPS1 |
| MOTA | 56 | 0 | ASP | 8 | 58.353 | 41.856 | 1.486 | | 3.32 |
| | | | | | | | | • | |

| MOTA | 57 | N | ILE | 9 | 56.124 | 41.944 | 1.328 | 1.00 19.03 | CPS1 |
|--------------|----------|-----|------------|----------|------------------|------------------|--------------------|--------------------------|--------------|
| ATOM | 58 | CA | ILE | 9 | 56.051 | 40.795 | 0.444 | 1.00 19.29 | CPS1 |
| ATOM | 59 | CB | ILE | 9 | 55.393 | 39.567 | 1.093 | 1.00 21.16 | CPS1 |
| MOTA | 60 | CG2 | ILE | 9 | 55.354 | 38.416 | 0.080 | 1.00 20.76 | CPS1 |
| MOTA | 61 | CG1 | ILE | 9 | 56.198 | 39.115 | 2.308 | 1.00 19.57 | CPS1 |
| MOTA | 62 | CD1 | ILE | 9 | 55.560 | 37.946 | 3.081 | 1.00 21.48 | CPS1 |
| MOTA | 63 | С | ILE | 9 | 55.161 | 41.304 | -0.683 | 1.00 20.60 | CPS1 |
| MOTA | 64 | 0 | ILE | 9 | 54.102 | 41.904 | -0.431 | 1.00 18.57 | CPS1 |
| MOTA | 65 | N | THR | 10 | 55.601 | 41.100 | -1.916 | 1.00 20.85 | CPS1 |
| ATOM | 66 | CA | THR | 10 | 54.828 | 41.556 | -3.064 | 1.00 22.77 | CPS1 |
| ATOM | 67 | CB | THR | 10 | 55.555 | 42.710 | -3.789 | 1.00 25.32 | CPS1 |
| MOTA | 68 | OG1 | THR | 10 | 55.699 | 43.816 | -2.889 | 1.00 26.50 | CPS1 |
| MOTA | 69 | CG2 | THR | 10 | 54.758 | 43.168 | -5.014 | 1.00 26.33 | CPS1 |
| MOTA | 70 | С | THR | 10 | 54.598 | 40.400 | -4.028 | 1.00 22.74 | CPS1 |
| MOTA | 71 | 0 | THR | 10 | 55.506 | 39.633 | -4.314 | 1.00 21.67 | CPS1 |
| MOTA | 72 | N | GLU | 11 | 53.359 | 40.270 | -4.495 | 1.00 24.96 | CPS1 |
| MOTA | 73 | CA | GLU | 11 | 52.993 | 39.223 | -5.445 | 1.00 25.76 | CPS1 |
| MOTA | 74 | CB | GLU | 11 | 51.475 | 38.995 | -5.394 | 1.00 28.49 | CPS1 |
| MOTA | 75 | CG | GLU | 11 | 50.969 | 37.968 | -6.383 | 1.00 31.23 | CPS1 |
| MOTA | 76 | CD | GLU | 11 | 49.445 | 37.895 | -6.440 | 1.00 34.90 | CPS1 |
| MOTA | 77 | | GLU | 11 | 48.773 | 38.865 | -6.019 | 1.00 33.91 | CPS1 |
| MOTA | 78 | | GLU | 11 | 48.923 | 36.867 | -6.926 | 1.00 35.55 | CPS1 |
| ATOM | 79 | C | GLU | 11 | 53.420 | 39.693 | -6.842 | 1.00 25.44 | CPS1 |
| ATOM | 80 | 0 | GLU | 11 | 53.000 | 40.761 | -7.293 | 1.00 24.85 | CPS1 |
| ATOM | 81 | N | LEU | 12 | 54.252 | 38.912 | -7.525 | 1.00 26.00 | CPS1 |
| MOTA | 82 | CA | LEU | 12 | 54.715 | 39.316 | -8.857 | 1.00 27.71 | CPS1 |
| ATOM | 83 | CB | LEU | 12 | 55.599 | 38.242 | -9.488 | 1.00 28.64 | CPS1 |
| MOTA | 84 | CG | LEU | 12 | 56.860 | 37.729 | -8.793 | 1.00 31.06 | CPS1 |
| ATOM | 85 | | LEU | 12 | 57.721 | 37.022 | -9.836 | 1.00 31.75 | CPS1 |
| ATOM | 86 | | LEU | 12 | 57.643 | 38.862 | -8.157 | 1.00 31.13 | CPS1 |
| ATOM | 87 | C | LEU | 12 | 53.557 | 39.608 | -9.810 | 1.00 28.75 | CPS1 |
| MOTA | 88 | 0 | LEU | 12 | 53.630 | | -10.631 | 1.00 28.32 | CPS1 |
| MOTA | 89 | N | ALA | 13 | 52.498 | 38.813 | -9.708 | 1.00 29.63 1.00 32.09 | CPS1 CPS1 |
| ATOM | 90 | CA | ALA | 13 | 51.330 50.281 | 38.987 37.918 | -10.565 -10.238 | 1.00 32.09 | CPS1 |
| MOTA | 91 92 | CB | ALA ALA | 13 13 | 50.732 | | -10.238 | 1.00 32.02 | CPS1 |
| ATOM ATOM | 93 | 0 | ALA | 13 | 50.732 | | -11.369 | 1.00 33.79 | CPS1 |
| ATOM | 93 94 | N | ARG | 14 | 50.732 | 40.864 | -9.160 | 1.00 34.46 | CPS1 |
| ATOM | 95 | CA | ARG | 14 | 50.188 | 42.178 | -8.846 | 1.00 35.63 | CPS1 |
| ATOM | 96 | CB | ARG | 14 | 50.170 | 42.380 | -7.330 | 1.00 38.10 | CPS1 |
| ATOM | 97 | CG | ARG | 14 | 48.818 | 42.770 | -6.772 | 1.00 41.02 | CPS1 |
| ATOM | 98 | CD | ARG | 14 | 48.815 | 44.197 | -6.276 | 1.00 42.88 | CPS1 |
| ATOM | 99 | NE | ARG | 14 | 49.762 | 44.395 | -5.183 | 1.00 43.99 | CPS1 |
| ATOM | 100 | CZ | ARG | 14 | 50.030 | 45.575 | | 1.00 45.35 | CPS1 |
| ATOM | 101 | | ARG | 14 | 49.420 | 46.670 | | 1.00 46.27 | CPS1 |
| MOTA | 102 | | ARG | 14 | 50.915 | 45.664 | | 1.00 44.46 | CPS1 |
| MOTA | 103 | С | ARG | 14 | 51.022 | 43.264 | | 1.00 36.31 | CPS1 |
| MOTA | 104 | ō | ARG | 14 | 50.484 | | -10.055 | 1.00 36.04 | CPS1 |
| ATOM | 105 | N | ILE | 15 | 52.340 | 43.095 | | 1.00 35.62 | CPS1 |
| ATOM | 106 | CA | ILE | 15 | 53.258 | 44.046 | -10.062 | 1.00 36.49 | CPS1 |
| ATOM | 107 | CB | ILE | 15 | 54.720 | 43.639 | | 1.00 34.84 | CPS1 |
| ATOM | 108 | | ILE | 15 | 55.666 | | -10.646 | 1.00 34.69 | CPS1 |
| ATOM | 109 | | ILE | 15 | 55.037 | 43.835 | | 1.00 32.18 | CPS1 |
| ATOM | 110 | | ILE | 15 | 54.936 | 45.275 | | 1.00 33.49 | CPS1 |
| ATOM | 111 | С | ILE | 15 | 52.995 | | -11.566 | 1.00 39.03 | CPS1 |
| ATOM | 112 | 0 | ILE | 15 | 53.103 | | -12.195 | 1.00 38.89 | CPS1 |
| ATOM | 113 | N | ALA | | 52.651 | | -12.141 | 1.00 41.54 | CPS1 |
| | | | | | | | | | |

| | | ~- | | | 50 000 | | | | |
|------|-----|-----|-----|----|--------|-------------|-----------------|-----------|------|
| ATOM | 114 | CA | ALA | 16 | 52.336 | 42.837 -13. | | 00 44.64 | CPS1 |
| ATOM | 115 | CB | ALA | 16 | 52.211 | 41.436 -14. | 018 1.0 | 00 44.42 | CPS1 |
| ATOM | 116 | C | ALA | 16 | 51.016 | 43.629 -13. | 784 1.0 | 00 46.09 | CPS1 |
| MOTA | 117 | 0 | ALA | 16 | 50.869 | 44.377 -14. | 746 1.1 | 00 47.05 | CPS1 |
| MOTA | 118 | N | SER | 17 | 50.064 | 43.425 ~12. | | 00 49.05 | CPS1 |
| MOTA | 119 | CA | SER | 17 | 48.752 | 44.076 -12. | | 00 51.73 | |
| | | | | | | | | | CPS1 |
| MOTA | 120 | CB | SER | 17 | 47.823 | 43.567 -11. | | 00 51.91 | CPS1 |
| ATOM | 121 | OG | SER | 17 | 47.472 | 42.208 -12. | .048 1. | 00 53.45 | CPS1 |
| ATOM | 122 | С | SER | 17 | 48.851 | 45.594 -12. | 854 1. | 00 53.68 | CPS1 |
| ATOM | 123 | 0 | SER | 17 | 48.310 | 46.316 -13 | 691 1. | 00 54.03 | CPS1 |
| ATOM | 124 | N | MET | 18 | 49.530 | 46.075 -11. | | 00 55.71 | CPS1 |
| ATOM | 125 | | MET | | | | | | |
| | | CA | | 18 | 49.697 | 47.511 -11. | | 00 57.69 | CPS1 |
| ATOM | 126 | CB | MET | 18 | 50.429 | 47.787 -10 | | 00 58.63 | CPS1 |
| ATOM | 127 | CG | MET | 18 | 49.679 | 47.357 -9 | .046 1. | 00 60.86 | CPS1 |
| ATOM | 128 | SD | MET | 18 | 50.678 | 47.547 -7 | .546 1 <i>.</i> | 00 64.39 | CPS1 |
| ATOM | 129 | CE | MET | 18 | 50.115 | 49.133 -6 | .944 1. | 00 63.23 | CPS1 |
| ATOM | 130 | С | MET | 18 | 50.489 | 48.126 -12 | .758 1. | 00 58.14 | CPS1 |
| ATOM | 131 | Ō | MET | 18 | 50.147 | 49.200 -13 | | 00 58.47 | CPS1 |
| ATOM | 132 | N | ALA | 19 | 51.545 | 47.440 -13 | | 00 58.63 | CPS1 |
| | | | | | | | | | |
| MOTA | 133 | CA | ALA | 19 | 52.393 | 47.930 -14 | | 00 59.73 | CPS1 |
| MOTA | 134 | CB | ALA | 19 | 53.432 | 46.881 -14 | | 00 58.94 | CPS1 |
| MOTA | 135 | C | ALA | 19 | 51.593 | 48.320 -15 | .490 1. | 00 61.14 | CPS1 |
| ATOM | 136 | 0 | ALA | 19 | 51.267 | 49.491 -15 | .679 1. | 00 61.35 | CPS1 |
| ATOM | 137 | N | GLY | 20 | 51.282 | 47.329 -16 | .322 1. | 00 62.81 | CPS1 |
| ATOM | 138 | CA | GLY | 20 | 50.537 | 47.568 -17 | | 00 64.34 | CPS1 |
| | | C | GLY | 20 | 49.331 | 48.486 -17 | | 00 65.24 | CPS1 |
| ATOM | 139 | | | | | | | | |
| MOTA | 140 | 0 | GLY | 20 | 49.010 | 49.210 -18 | | 00 65.67 | CPS1 |
| ATOM | 141 | N | ARG | 21 | 48.660 | 48.459 -16 | | 00 65.86 | CPS1 |
| ATOM | 142 | CA | ARG | 21 | 47.485 | 49.295 -16 | .081 1. | 00 66.76 | CPS1 |
| ATOM | 143 | CB | ARG | 21 | 46.595 | 48.672 -14 | .996 1. | 00 68.01 | CPS1 |
| ATOM | 144 | CG | ARG | 21 | 45.294 | 49.417 -14 | .698 1. | 00 70.30 | CPS1 |
| MOTA | 145 | CD | ARG | 21 | 44.482 | 49.731 -15 | .959 1. | 00 72.22 | CPS1 |
| MOTA | 146 | NE | ARG | 21 | 44.987 | 50.908 -16 | | 00 73.68 | CPS1 |
| | | | | | | | | | CPS1 |
| MOTA | 147 | CZ | ARG | 21 | 44.415 | 51.435 -17 | | 00 74.14 | |
| MOTA | 148 | | ARG | 21 | 43.314 | 50.891 -18 | | 00 74.30 | CPS1 |
| ATOM | 149 | NH2 | ARG | 21 | 44.941 | 52.510 -18 | .324 1. | 00 74.39 | CPS1 |
| ATOM | 150 | C | ARG | 21 | 47.862 | 50.728 -15 | .703 1. | 00 66.35 | CPS1 |
| ATOM | 151 | 0 | ARG | 21 | 47.312 | 51.296 -14 | .759 1. | 00 66.83 | CPS1 |
| ATOM | 152 | N | GLN | 22 | 48.803 | 51.304 -16 | .450 1. | 00 65.49 | CPS1 |
| ATOM | 153 | CA | GLN | 22 | 49.263 | 52.676 -16 | | 00 64.27 | CPS1 |
| | | | GLN | 22 | 50.068 | 52.755 -14 | | 00 64.78 | CPS1 |
| ATOM | 154 | CB | | | | | | | CPS1 |
| ATOM | 155 | CG | GLN | 22 | 49.187 | 52.941 -13 | | 00 66.23 | |
| ATOM | 156 | CD | GLN | 22 | 49.924 | 52.717 -12 | | 00 67.13 | CPS1 |
| ATOM | 157 | OE1 | GLN | 22 | 50.946 | 53.353 -12 | .097 1. | 00 67.87 | CPSI |
| ATOM | 158 | NE2 | GLN | 22 | 49.401 | 51.812 -11 | .544 1. | 00 67.13 | CPS1 |
| MOTA | 159 | С | GLN | 22 | 50.086 | 53.230 -17 | .393 1. | 00 62.83 | CPS1 |
| MOTA | 160 | ō | GLN | 22 | 49.559 | 53.962 -18 | | 00 63.71 | CPS1 |
| ATOM | | | GLY | 23 | 51.368 | 52.878 -17 | | 00 59.93 | CPS1 |
| | 161 | И | | | | | | | |
| MOTA | 162 | CA | GLY | 23 | 52.215 | 53.360 -18 | | 00 54.65 | CPS1 |
| MOTA | 163 | С | GLY | 23 | 53.259 | 54.325 -18 | | 00 51.39 | CPS1 |
| MOTA | 164 | 0 | GLY | 23 | 53.852 | 55.099 -18 | | 00 50.70 | CPS1 |
| ATOM | 165 | N | ARG | 24 | 53.474 | 54.268 -16 | .694 1. | 00 47.29 | CPS1 |
| ATOM | 166 | CA | ARG | 24 | 54.433 | 55.121 -16 | | 00 42.63 | CPS1 |
| ATOM | 167 | CB | ARG | 24 | 53.798 | 56.490 -15 | | 00 45.51 | CPS1 |
| | | | | | | 57.512 -15 | | 00 48.36 | CPS1 |
| ATOM | 168 | CG | ARG | 24 | 54.684 | | | .00 50.96 | CPS1 |
| ATOM | 169 | CD | ARG | 24 | 54.194 | 58.925 -15 | | | |
| ATOM | 170 | NE | ARG | 24 | 52.773 | 59.092 -15 | .108 1 | .00 53.61 | CPS1 |
| | | | | | | | | | |

| ATOM | 171 | CZ | ARG | 24 | 52.092 | 60.215 -15.320 | 1.00 54.82 | CPS1 |
|--------------|------------|-----|-----|----------|--------|--------------------------------|------------|--------------|
| ATOM | 172 | NHl | ARG | 24 | 52.704 | 61.281 -15.824 | 1.00 55.59 | CPS1 |
| ATOM | 173 | NH2 | ARG | 24 | 50.796 | 60.270 -15.039 | 1.00 55.48 | CPS1 |
| ATOM | 174 | C | ARG | 24 | 54.842 | 54.480 -14.673 | 1.00 38.31 | CPS1 |
| ATOM | 175 | 0 | ARG | 24 | 55.617 | 55.045 -13.906 | 1.00 35.06 | CPS1 |
| ATOM | 176 | N | PHE | 25 | 54.338 | 53.279 -14.420 | 1.00 34.51 | CPS1 |
| ATOM | 177 | CA | PHE | 25 | 54.630 | 52.585 -13.166 | 1.00 32.21 | CPS1 |
| ATOM | 178 | CB | PHE | 25 | 53.805 | 51.298 -13.074 | 1.00 33.02 | CPS1 |
| ATOM | 179 | CG | PHE | 25 | 54.016 | 50.536 -11.797 | 1.00 33.13 | CPS1 |
| MOTA | 180 | CD1 | PHE | 25 | 54.917 | 49.482 -11.741 | 1.00 33.65 | CPS1 |
| ATOM | 181 | CD2 | PHE | 25 | 53.323 | 50.889 -10.642 | 1.00 34.84 | CPS1 |
| MOTA | 182 | CEl | | 25 | 55.129 | 48.784 -10.553 | 1.00 33.64 | CPS1 |
| ATOM | 183 | | PHE | 25 | 53.527 | 50.201 -9.450 | 1.00 34.46 | CPS1 |
| ATOM | 184 | CZ | PHE | 25 | 54.432 | 49.146 -9.405 | 1.00 34.16 | CPS1 |
| ATOM | 185 | C | PHE | 25 | 56.103 | 52.273 -12.902 | 1.00 29.41 | CPS1 |
| ATOM | 186 | ō | PHE | 25 | 56.632 | 52.657 -11.862 | 1.00 29.18 | CPS1 |
| ATOM | 187 | N | ALA | 26 | 56.771 | 51.585 -13.826 | 1.00 26.94 | CPS1 |
| MOTA | 188 | CA | ALA | 26 | 58.177 | 51.245 -13.621 | 1.00 25.77 | CPS1 |
| MOTA | 189 | CB | ALA | 26 | 58.702 | 50.403 -14.785 | 1.00 25.23 | CPS1 |
| ATOM | 190 | C | ALA | 26 | 59.043 | 52.480 -13.459 | 1.00 25.25 | CPS1 |
| ATOM | 191 | 0 | ALA | 26 | 59.955 | 52.511 -12.632 | 1.00 23.55 | CPS1 |
| ATOM | 192 | Ŋ | GLU | 27 | 58.757 | 53.502 -14.260 | 1.00 24.05 | CPS1 |
| ATOM | 193 | CA | GLU | 27 | 59.537 | 54.726 -14.210 | 1.00 25.73 | CPS1 |
| ATOM | 194 | CB | GLU | 27 | 59.225 | 55.589 -15.436 | 1.00 25.75 | CPS1 |
| ATOM | 195 | CG | GLU | 27 | 59.695 | 54.987 -16.750 | 1.00 26.79 | CPS1 |
| ATOM | 196 | CD | GLU | 27 | 58.896 | 53.770 -17.202 | 1.00 28.70 | CPS1 |
| ATOM | 197 | | GLU | 27 | 57.680 | 53.695 -16.908 | 1.00 20.20 | CPS1 |
| ATOM | 198 | | GLU | 27 | 59.481 | 52.894 -17.877 | 1.00 29.45 | CPS1 |
| ATOM | 199 | C | GLU | 27 | 59.315 | 55.519 -12.924 | 1.00 26.62 | CPS1 |
| MOTA | 200 | 0 | GLU | 27 | 60.158 | 56.322 -12.532 | 1.00 20.02 | CPS1 |
| ATOM | 201 | Ŋ | ARG | 28 | 58.179 | 55.312 -12.272 | 1.00 27.44 | CPS1 |
| ATOM | 202 | CA | ARG | 28 | 57.924 | 56.002 -11.014 | 1.00 28.43 | CPS1 |
| | 203 | CB | ARG | 28 | 56.422 | 56.062 -10.727 | 1.00 20.45 | CPS1 |
| ATOM ATOM | 204 | CG | ARG | 28 | 55.736 | 57.322 -11.243 | 1.00 31.73 | CPS1 |
| ATOM | 205 | CD | ARG | 28 | 54.229 | 57.195 -11.093 | 1.00 38.22 | CPS1 |
| ATOM | 205 | NE | ARG | 28 | 53.891 | 56.446 -9.885 | 1.00 41.54 | CPS1 |
| | 207 | CZ | ARG | 28 | 53.088 | 55.387 -9.869 | 1.00 47.55 | CPS1 |
| ATOM | 207 | | ARG | 28 | 52.534 | 54.953 -11.000 | 1.00 47.33 | CPS1 |
| ATOM | 209 | | ARG | 28 | 52.855 | 54.751 -8.726 | 1.00 49.13 | CPS1 |
| ATOM | | C | ARG | 28 | 58.629 | 55.267 -9.877 | 1.00 49.13 | CPS1 |
| ATOM | 210 | 0 | ARG | 28 | 59.086 | 55.885 -8.928 | 1.00 27.28 | CPS1 |
| ATOM | 211 212 | N | ILE | 28 29 | 58.729 | 53.944 -9.985 | 1.00 27.20 | CPS1 |
| ATOM | | | | 29 | 59.363 | 53.137 -8.938 | 1.00 26.04 | CPS1 |
| MOTA | 213 | CA | ILE | | | | 1.00 26.47 | CPS1 |
| ATOM | 214 | CB | ILE | 29 | 58.901 | 51.657 -9.004 50.865 -7.858 | 1.00 28.14 | CPS1 |
| ATOM | 215 | | ILE | 29 | 59.520 | | 1.00 25.14 | CPS1 |
| ATOM | 216 | | ILE | 29 | 57.374 | | 1.00 28.72 | CPS1 |
| ATOM | 217 | | ILE | 29 | 56.722 | 52.214 -7.796 | | CPS1 |
| MOTA | 218 | C | ILE | 29 | 60.888 | 53.122 -8.980 | 1.00 25.23 | CPS1 |
| MOTA | 219 | 0 | ILE | 29 | 61.549 | 53.123 -7.934 | 1.00 25.57 | CPS1 |
| MOTA | 220 | N | LEU | 30 | 61.445 | 53.119 -10.188 | 1.00 23.44 | CPS1 |
| ATOM | 221 | CA | LEU | 30 | 62.885 | 53.031 -10.371 | 1.00 22.74 | |
| ATOM | 222 | CB | LEU | 30 | 63.185 | 52.029 -11.487 | 1.00 22.73 | CPS1 |
| ATOM | 223 | CG | LEU | 30 | 62.509 | 50.656 -11.381 | 1.00 22.89 | CPS1 CPS1 |
| MOTA | 224 | | LEU | 30 | 62.817 | 49.861 -12.635 | 1.00 22.68 | |
| MOTA | 225 | | LEU | 30 | 63.004 | 49.922 -10.126 | 1.00 22.78 | CPS1 |
| MOTA | 226 | C | LEU | 30 | 63.590 | 54.344 -10.686 | 1.00 23.94 | CPS1 |
| ATOM | 227 | 0 | LEU | 30 | 63.027 | 55.228 -11.336 | 1.00 23.90 | CPS1 |
| | | | | | | | | |

| ATOM | 228 | N | THR | 31 | 64.830 | 54.451 | -10.224 | 1.00 24.75 | CPS1 |
|------|------------|-----------|------------|----------|--------|--------|---------|--------------------------|------|
| ATOM | 229 | CA | THR | 31 | 65.643 | 55.636 | -10.461 | 1.00 25.03 | CPS1 |
| MOTA | 230 | CB | THR | 31 | 66.787 | 55.749 | -9.457 | 1.00 26.35 | CPS1 |
| ATOM | 231 | OG1 | THR | 31 | 67.725 | 54.692 | -9.695 | 1.00 26.00 | CPS1 |
| MOTA | 232 | CG2 | THR | 31 | 66.261 | 55.671 | -8.031 | 1.00 26.75 | CPS1 |
| MOTA | 233 | C | THR | 31 | 66.271 | 55.469 | -11.832 | 1.00 24.44 | CPS1 |
| ATOM | 234 | 0 | THR | 31 | 66.163 | 54.416 | -12.441 | 1.00 22.68 | CPS1 |
| ATOM | 235 | N | ARG | 32 | 66.963 | 56.503 | -12.293 | 1.00 25.91 | CPS1 |
| ATOM | 236 | CA | ARG | 32 | 67.607 | 56.458 | -13.603 | 1.00 26.68 | CPS1 |
| ATOM | 237 | CB | ARG | 32 | 68.342 | 57.780 | -13.848 | 1.00 26.75 | CPS1 |
| ATOM | 238 | CG | ARG | 32 | 68.970 | 57.939 | -15.236 | 1.00 29.21 | CPS1 |
| MOTA | 239 | CD | ARG | 32 | 69.551 | | -15.344 | 1.00 29.81 | CPS1 |
| MOTA | 240 | NE | ARG | 32 | 70.015 | | -16.684 | 1.00 32.75 | CPS1 |
| ATOM | 241 | CZ | ARG | 32 | 71.129 | | -17.254 | 1.00 34.02 | CPS1 |
| ATOM | 242 | NH1 | | 32 | 71.916 | | -16.606 | 1.00 33.55 | CPS1 |
| ATOM | 243 | NH2 | | 32 | 71.476 | | -18.464 | 1.00 31.94 | CPS1 |
| ATOM | 244 | C | ARG | 32 | 68.572 | | -13.728 | 1.00 26.02 | CPS1 |
| MOTA | 245 | 0 | ARG | 32 | 68.539 | | -14.721 | 1.00 25.46 | CPS1 |
| ATOM | 246 | N | SER | 33 | 69.422 | | -12.721 | 1.00 26.77 | CPS1 |
| ATOM | 247 | CA | SER | 33 | 70.390 | | -12.725 | 1.00 28.08 | CPS1 |
| ATOM | 248 | CB | SER | 33 | 71.277 | | -11.473 | 1.00 31.22 | CPS1 |
| ATOM | 249 | OG | SER | 33 | 72.112 | | -11.481 | 1.00 38.13 | CPS1 |
| ATOM | 250 | C | SER | 33 | 69.686 | | -12.772 | 1.00 27.50 | CPS1 |
| ATOM | 251 | ō | SER | 33 | 70.113 | | -13.487 | 1.00 28.27 | CPS1 |
| ATOM | 252 | И | GLU | 34 | 68.613 | | -11.998 | 1.00 25.27 | CPS1 |
| ATOM | 253 | CA | GLU | 34 | 67.857 | | -11.970 | 1.00 25.33 | CPS1 |
| ATOM | 254 | CB | GLU | 34 | 66.842 | | -10.822 | 1.00 25.24 | CPS1 |
| ATOM | 255 | CG | GLU | 34 | 67.531 | 51.247 | -9.455 | 1.00 24.32 | CPS1 |
| ATOM | 256 | CD | GLU | 34 | 66.575 | 51.424 | -8.280 | 1.00 26.32 | CPS1 |
| ATOM | 257 | | GLU | 34 | 66.860 | 50.849 | -7.202 | 1.00 24.86 | CPS1 |
| MOTA | 258 | OE2 | GLU | 34 | 65.557 | 52.145 | -8.423 | 1.00 25.42 | CPS1 |
| ATOM | 259 | C | GLU | 34 | 67.167 | | -13.302 | 1.00 25.42 | CPS1 |
| ATOM | 260 | 0 | GLU | 34 | 67.113 | | -13.767 | 1.00 25.37 | CPS1 |
| ATOM | 261 | Ŋ | LEU | 35 | 66.649 | | -13.919 | 1.00 25.65 | CPS1 |
| ATOM | 262 | CA | LEU | 35 | 65.978 | | -15.209 | 1.00 25.43 | CPS1 |
| ATOM | 263 | CB | LEU | 35 | 65.362 | | -15.626 | 1.00 24.81 | CPS1 |
| ATOM | 264 | CG | LEU | 35 | 64.044 | | -14.936 | 1.00 25.80 | CPS1 |
| ATOM | 265 | | LEU | 35 | 63.598 | | -15.354 | 1.00 24.72 | CPS1 |
| ATOM | 266 | | LEU | 35 | 62.980 | | -15.320 | 1.00 24.72 | CPS1 |
| ATOM | 267 | CDZ | LEU | 35 | 66.961 | | -16.278 | 1.00 25.60 | CPS1 |
| ATOM | 268 | 0 | LEU | 35 | 66.608 | | -17.139 | 1.00 25.96 | CPS1 |
| ATOM | 269 | И | ASP | 36 | 68.189 | | -16.213 | 1.00 26.39 | CPS1 |
| | 270 | | ASP | 36 | 69.221 | | -17.176 | 1.00 28.65 | CPS1 |
| MOTA | | CA | | 36 | 70.549 | | -16.814 | 1.00 30.67 | CPS1 |
| MOTA | 271 | CB | ASP ASP | 36 | 70.543 | | -17.834 | 1.00 34.97 | CPS1 |
| ATOM | 272 273 | CG OD1 | ASP | 36 | 71.337 | | -19.045 | 1.00 36.35 | CPS1 |
| ATOM | | | | | | | -17.421 | 1.00 38.35 | CPS1 |
| ATOM | 274 | | ASP | 36 36 | 72.780 | | -17.176 | 1.00 29.59 | CPS1 |
| ATOM | 275 | C | ASP | 36 | 69.374 | | | 1.00 29.62 | CPS1 |
| MOTA | 276 | 0 | ASP | 36 | 69.510 | | -18.229 | 1.00 29.82 | CPS1 |
| ATOM | 277 | N | GLN | 37 | 69.331 | | -15.987 | 1.00 29.18 | CPS1 |
| ATOM | 278 | CA | GLN | 37 | 69.446 | | -15.860 | 1.00 27.84 | CPS1 |
| ATOM | 279 | CB | GLN | 37 | 69.737 | | -14.404 | | CPS1 |
| ATOM | 280 | CG | GLN | 37 | 70.983 | | -13.850 | 1.00 32.00 1.00 34.39 | CPS1 |
| ATOM | 281 | CD | GLN | 37 | 71.075 | | -12.348 | | CPS1 |
| MOTA | 282 | | GLN | 37 | 71.087 | | -11.805 | 1.00 34.90 | CPS1 |
| MOTA | 283 | | GLN | 37 | 71.142 | | -11.662 | 1.00 34.48 | CPS1 |
| MOTA | 284 | С | GLN | 37 | 68.156 | 47.335 | -16.301 | 1.00 27.75 | CPSI |
| | | | | | | | | | |

| MOTA | 285 | 0 | GLN | 37 | 68.183 | 46.328 -17.012 | 1.00 27.75 | CPS1 |
|------|-------------|-----|-----|----|--------|----------------|------------|------|
| ATOM | 286 | N | TYR | 38 | 67.031 | 47.885 -15.858 | 1.00 26.28 | CPS1 |
| ATOM | 287 | CA | TYR | 38 | 65.705 | 47.352 -16.167 | 1.00 25.28 | CPS1 |
| MOTA | 288 | CB | TYR | 38 | 64.657 | 48.251 -15.500 | 1.00 25.99 | CPS1 |
| MOTA | 289 | CG | TYR | 38 | 63.213 | 47.908 -15.772 | 1.00 26.20 | CPS1 |
| MOTA | 290 | | TYR | 38 | 62.468 | 48.648 -16.688 | 1.00 26.19 | CPS1 |
| ATOM | 291 | CEl | TYR | 38 | 61.121 | 48.385 -16.903 | 1.00 26.29 | CPS1 |
| MOTA | 292 | CD2 | TYR | 38 | 62.567 | 46.881 -15.074 | 1.00 26.31 | CPS1 |
| ATOM | 293 | CE2 | TYR | 38 | 61.219 | 46.611 -15.280 | 1.00 25.67 | CPS1 |
| ATOM | 294 | CZ | TYR | 38 | 60.501 | 47.370 -16.200 | 1.00 28.03 | CPS1 |
| ATOM | 295 | OH | TYR | 38 | 59.166 | 47.120 -16.428 | 1.00 27.03 | CPS1 |
| ATOM | 296 | С | TYR | 38 | 65.420 | 47.208 -17.668 | 1.00 26.52 | CPS1 |
| ATOM | 297 | 0 | TYR | 38 | 64.912 | 46.175 -18.122 | 1.00 23.95 | CPS1 |
| ATOM | 298 | N | TYR | 39 | 65.756 | 48.235 -18.440 | 1.00 26.98 | CPS1 |
| ATOM | 299 | CA | TYR | 39 | 65.502 | 48.193 -19.880 | 1.00 29.18 | CPS1 |
| ATOM | 300 | CB | TYR | 39 | 65.757 | 49.579 -20.488 | 1.00 28.06 | CPS1 |
| ATOM | 301 | CG | TYR | 39 | 64.725 | 50.615 -20.060 | 1.00 27.09 | CPS1 |
| ATOM | 302 | CD1 | TYR | 39 | 63.365 | 50.313 -20.080 | 1.00 26.88 | CPS1 |
| MOTA | 303 | CE1 | TYR | 39 | 62.402 | 51.252 -19.691 | 1.00 26.96 | CPS1 |
| MOTA | 304 | CD2 | TYR | 39 | 65.109 | 51.890 -19.641 | 1.00 26.42 | CPS1 |
| MOTA | 305 | CE2 | TYR | 39 | 64.154 | 52.841 -19.245 | 1.00 27.05 | CPS1 |
| ATOM | 306 | cz | TYR | 39 | 62.806 | 52.510 -19.274 | 1.00 26.67 | CPS1 |
| ATOM | 307 | OH | TYR | 39 | 61.856 | 53.426 -18.876 | 1.00 27.91 | CPS1 |
| ATOM | 308 | C | TYR | 39 | 66.279 | 47.108 -20.641 | 1.00 31.26 | CPS1 |
| ATOM | 309 | 0 | TYR | 39 | 65.899 | 46.727 -21.750 | 1.00 32.43 | CPS1 |
| ATOM | 310 | N | GLU | 40 | 67.351 | 46.597 -20.046 | 1.00 32.52 | CPS1 |
| ATOM | 311 | CA | GLU | 40 | 68.150 | 45.555 -20.690 | 1.00 33.92 | CPS1 |
| ATOM | 312 | CB | GLU | 40 | 69.602 | 45.621 -20.207 | 1.00 35.68 | CPS1 |
| ATOM | 313 | CG | GLU | 40 | 70.340 | 46.890 -20.579 | 1.00 38.76 | CPS1 |
| ATOM | 314 | CD | GLU | 40 | 70.370 | 47.130 -22.079 | 1.00 41.13 | CPS1 |
| ATOM | 315 | OE1 | GLU | 40 | 70.557 | 46.153 -22.835 | 1.00 43.88 | CPS1 |
| MOTA | 316 | OE2 | GLU | 40 | 70.220 | 48.297 -22.501 | 1.00 41.69 | CPS1 |
| MOTA | 317 | С | GLU | 40 | 67.616 | 44.147 -20.419 | 1.00 34.35 | CPS1 |
| MOTA | 318 | 0 | GLU | 40 | 68.089 | 43.177 -21.008 | 1.00 33.76 | CPS1 |
| MOTA | 319 | N | LEU | 41 | 66.626 | 44.036 -19.541 | 1.00 33.60 | CPS1 |
| MOTA | 320 | CA | LEU | 41 | 66.080 | 42.733 -19.176 | 1.00 34.81 | CPS1 |
| ATOM | 321 | CB | LEU | 41 | 65.658 | 42.757 -17.702 | 1.00 33.78 | CPS1 |
| MOTA | 322 | CG | LEU | 41 | 66.725 | 43.183 -16.690 | 1.00 33.47 | CPS1 |
| ATOM | 323 | CD1 | LEU | 41 | 66.084 | 43.291 -15.309 | 1.00 33.49 | CPS1 |
| ATOM | 324 | CD2 | LEU | 41 | 67.879 | 42.188 -16.678 | 1.00 33.26 | CPS1 |
| ATOM | 325 | C | LEU | 41 | 64.910 | 42.221 -20.013 | 1.00 35.00 | CPS1 |
| ATOM | 326 | 0 | LEU | 41 | 64.199 | 42.992 -20.654 | 1.00 34.86 | CPS1 |
| ATOM | 327 | N | SER | 42 | 64.713 | 40.904 -19.984 | 1.00 36.21 | CPS1 |
| ATOM | 328 | CA | SER | 42 | 63.615 | 40.271 -20.709 | 1.00 37.02 | CPS1 |
| MOTA | 329 | CB | SER | 42 | 63.788 | 38.752 -20.716 | 1.00 37.19 | CPS1 |
| MOTA | 330 | OG | SER | 42 | 63.601 | 38.228 -19.413 | 1.00 37.95 | CPS1 |
| MOTA | 331 | C | SER | 42 | 62.321 | 40.628 -19.986 | 1.00 37.67 | CPS1 |
| MOTA | 332 | 0 | SER | 42 | 62.355 | 41.124 -18.856 | 1.00 37.09 | CPS1 |
| MOTA | 333 | N | GLU | 43 | 61.180 | 40.378 -20.618 | 1.00 37.74 | CPS1 |
| ATOM | 334 | CA | GLU | 43 | 59.917 | 40.705 -19.970 | 1.00 39.67 | CPS1 |
| ATOM | 33 5 | CB | GLU | 43 | 58.716 | 40.282 -20.829 | 1.00 42.30 | CPS1 |
| ATOM | 336 | CG | GLU | 43 | 57.421 | 40.990 -20.417 | 1.00 46.74 | CPS1 |
| ATOM | 337 | CD | GLU | 43 | 56.177 | 40.466 -21.122 | 1.00 49.57 | CPS1 |
| ATOM | 338 | OEl | GLU | 43 | 56.253 | 40.155 -22.333 | 1.00 51.74 | CPS1 |
| ATOM | 339 | OE2 | GLU | 43 | 55.116 | 40.384 -20.465 | 1.00 50.82 | CPS1 |
| ATOM | 340 | C | GLU | 43 | 59.833 | 40.012 -18.611 | 1.00 38.42 | CPS1 |
| ATOM | 341 | 0 | GLU | 43 | 59.425 | 40.619 -17.623 | 1.00 37.06 | CPS1 |
| | | | | | | | | |

| ATOM | 342 | N | LYS | 44 | 60.223 | 38.743 -18.567 | 1.00 37.89 | anai |
|------|-----|-----|-----|----|--------|----------------|--------------|------|
| ATOM | 343 | | LYS | 44 | | 37.985 -17.318 | | CPS1 |
| | | CA | | | 60.176 | | | CPS1 |
| ATOM | 344 | CB | LYS | 44 | 60.566 | 36.525 -17.562 | | CPS1 |
| ATOM | 345 | CG | LYS | 44 | 60.777 | 35.706 -16.292 | | CPS1 |
| ATOM | 346 | CD | LYS | 44 | 60.766 | 34.214 -16.594 | | CPS1 |
| MOTA | 347 | CE | LYS | 44 | 61.613 | 33.425 -15.603 | 1.00 47.94 | CPS1 |
| MOTA | 348 | ΝZ | LYS | 44 | 63.073 | 33.691 -15.805 | 1.00 50.56 | CPS1 |
| MOTA | 349 | C | LYS | 44 | 61.086 | 38.587 -16.257 | 1.00 37.33 | CPS1 |
| ATOM | 350 | 0 | LYS | 44 | 60.661 | 38.823 -15.127 | 1.00 36.33 | CPS1 |
| ATOM | 351 | N | ARG | 45 | 62.338 | 38.835 -16.625 | 1.00 36.56 | CPS1 |
| ATOM | 352 | CA | ARG | 45 | 63.310 | 39.403 -15.695 | | CPS1 |
| ATOM | 353 | CB | ARG | 45 | 64.700 | 39.412 -16.333 | | CPS1 |
| MOTA | 354 | CG | ARG | 45 | 65.356 | 38.041 -16.385 | | CPS1 |
| MOTA | | | ARG | 45 | | | | |
| | 355 | CD | | | 65.840 | 37.633 -15.008 | | CPS1 |
| ATOM | 356 | NE | ARG | 45 | 66.842 | 38.569 -14.498 | | CPS1 |
| ATOM | 357 | CZ | ARG | 45 | 66.700 | 39.307 -13.399 | | CPS1 |
| ATOM | 358 | | ARG | 45 | 65.593 | 39.226 -12.672 | | CPS1 |
| ATOM | 359 | | ARG | 45 | 67.666 | 40.140 -13.033 | | CPS1 |
| ATOM | 360 | C | ARG | 45 | 62.920 | 40.807 -15.254 | 1.00 34.51 | CPS1 |
| MOTA | 361 | 0 | ARG | 45 | 63.182 | 41.200 -14.120 | 1.00 33.99 | CPS1 |
| MOTA | 362 | N | LYS | 46 | 62.294 | 41.565 -16.148 | 3 1.00 32.94 | CPS1 |
| ATOM | 363 | CA | LYS | 46 | 61.857 | 42.911 -15.802 | 1.00 32.28 | CPS1 |
| ATOM | 364 | CB | LYS | 46 | 61.165 | 43.580 -16.990 | 1.00 32.34 | CPS1 |
| ATOM | 365 | CG | LYS | 46 | 62.109 | 44.110 -18.051 | 1.00 32.52 | CPS1 |
| MOTA | 366 | CD | LYS | 46 | 61.327 | 44.905 -19.113 | 3 1.00 33.61 | CPS1 |
| MOTA | 367 | CE | LYS | 46 | 62.262 | 45.515 -20.153 | L 1.00 34.98 | CPS1 |
| ATOM | 368 | NZ | LYS | 46 | 61.505 | 46.250 -21.21 | | CPS1 |
| ATOM | 369 | C | LYS | 46 | 60.888 | 42.868 -14.623 | | CPS1 |
| ATOM | 370 | ō | LYS | 46 | 61.002 | 43.655 -13.684 | | CPS1 |
| ATOM | 371 | N | ASN | 47 | 59.937 | 41.942 -14.672 | | CPS1 |
| ATOM | 372 | CA | ASN | 47 | 58.951 | 41.806 -13.606 | | CPS1 |
| MOTA | | CB | ASN | 47 | 57.886 | 40.773 -14.013 | | CPS1 |
| | 373 | | ASN | 47 | | 40.449 -12.885 | | CPS1 |
| ATOM | 374 | CG | | | 56.914 | | | CPS1 |
| ATOM | 375 | | ASN | 47 | 57.020 | 39.401 -12.246 | | CPS1 |
| ATOM | 376 | | ASN | 47 | 55.969 | 41.346 -12.63 | | |
| ATOM | 377 | C | ASN | 47 | 59.608 | 41.424 -12.27 | | CPS1 |
| ATOM | 378 | 0 | ASN | 47 | 59.252 | 41.971 -11.23 | | CPS1 |
| MOTA | 379 | N | GLU | 48 | 60.568 | 40.503 -12.30 | | CPS1 |
| ATOM | 380 | CA | GLU | 48 | 61.265 | 40.064 -11.09 | | CPS1 |
| ATOM | 381 | CB | GLU | 48 | 62.172 | 38.870 -11.41 | | CPS1 |
| ATOM | 382 | CG | GLU | 48 | 61.417 | 37.675 -12.00 | | CPS1 |
| ATOM | 383 | CD | GLU | 48 | 62.338 | 36.589 -12.55 | | CPS1 |
| ATOM | 384 | OE1 | GLU | 48 | 61.815 | 35.595 -13.10 | 6 1.00 38.39 | CPS1 |
| MOTA | 385 | OE2 | GLU | 48 | 63.577 | 36.727 -12.43 | 4 1.00 38.18 | CPS1 |
| MOTA | 386 | C | GLU | 48 | 62.101 | 41.201 -10.49 | 8 1.00 26.11 | CPS1 |
| ATOM | 387 | 0 | GLU | 48 | 62.132 | 41.416 -9.27 | 1 1.00 22.48 | CPS1 |
| ATOM | 388 | N | PHE | 49 | 62.792 | 41.919 -11.37 | 7 1.00 23.64 | CPS1 |
| ATOM | 389 | CA | PHE | 49 | 63.628 | 43.042 -10.97 | 6 1.00 24.48 | CPS1 |
| ATOM | 390 | СВ | PHE | 49 | 64.356 | 43.591 -12.19 | | CPS1 |
| MOTA | 391 | CG | PHE | 49 | 65.252 | 44.754 -11.90 | | CPS1 |
| | | | PHE | 49 | | 44.552 -11.57 | | CPS1 |
| ATOM | 392 | | | | 66.591 | | | CPS1 |
| ATOM | 393 | | PHE | 49 | 64.771 | 46.052 -11.98 | | CPS1 |
| ATOM | 394 | | PHE | 49 | 67.438 | 45.632 -11.32 | | CPS1 |
| MOTA | 395 | | PHE | 49 | 65.601 | 47.137 -11.74 | | |
| ATOM | 396 | CZ | PHE | 49 | 66.938 | 46.933 -11.41 | | CPS1 |
| MOTA | 397 | C | PHE | 49 | 62.777 | | | CPS1 |
| MOTA | 398 | 0 | PHE | 49 | 63.124 | 44.721 -9.32 | 3 1.00 24.30 | CPS1 |

| MOTA | 399 | N | LEU | 50 | 61.672 | 44.476 | -11.029 | 1.00 22.90 | CPS1 |
|------|-----|-----|-----|----------|--------|--------|---------|------------|------|
| MOTA | 400 | CA | LEU | 50 | 60.795 | | -10.557 | 1.00 23.71 | CPS1 |
| ATOM | 401 | CB | LEU | 50 | 59.732 | 45.836 | -11.617 | 1.00 24.35 | CPS1 |
| ATOM | 402 | CG | LEU | 50 | 58.714 | 46.928 | -11.325 | 1.00 25.33 | CPS1 |
| ATOM | 403 | CD1 | LEU | 50 | 59.403 | 48.253 | -11.010 | 1.00 24.88 | CPS1 |
| MOTA | 404 | CD2 | LEU | 50 | 57.805 | 47.055 | -12.536 | 1.00 25.38 | CPS1 |
| MOTA | 405 | С | LEU | 50 | 60.132 | 45.138 | -9.236 | 1.00 23.44 | CPS1 |
| MOTA | 406 | 0 | LEU | 50 | 60.011 | 45.957 | -8.322 | 1.00 22.54 | CPS1 |
| MOTA | 407 | N | ALA | 51 | 59.698 | 43.884 | -9.148 | 1.00 22.99 | CPS1 |
| MOTA | 408 | CA | ALA | 51 | 59.056 | 43.399 | -7.929 | 1.00 23.20 | CPS1 |
| ATOM | 409 | CB | ALA | 51 | 58.581 | 41.959 | -8.123 | 1.00 23.60 | CPS1 |
| ATOM | 410 | C | ALA | 51 | 60.034 | 43.476 | -6.754 | 1.00 21.98 | CPS1 |
| ATOM | 411 | o | ALA | 51 | 59.655 | 43.884 | -5.653 | 1.00 21.38 | CPS1 |
| | | | GLY | 52 | | | | | |
| ATOM | 412 | N | | 52 52 | 61.284 | 43.089 | -6.998 | 1.00 21.48 | CPS1 |
| ATOM | 413 | CA | GLY | | 62.297 | 43.120 | -5.951 | 1.00 22.37 | CPS1 |
| ATOM | 414 | C | GLY | 52 | 62.585 | 44.523 | -5.460 | 1.00 22.17 | CPS1 |
| ATOM | 415 | 0 | GLY | 52 | 62.715 | 44.764 | -4.256 | 1.00 21.91 | CPS1 |
| ATOM | 416 | N | ARG | 53 | 62.675 | 45.461 | -6.402 | 1.00 23.24 | CPS1 |
| ATOM | 417 | CA | ARG | 53 | 62.933 | 46.862 | -6.076 | 1.00 23.63 | CPS1 |
| ATOM | 418 | CB | ARG | 53 | 63.169 | 47.654 | -7.364 | 1.00 25.69 | CPS1 |
| MOTA | 419 | CG | ARG | 53 | 64.546 | 48.242 | -7.490 | 1.00 29.63 | CPS1 |
| MOTA | 420 | CD | ARG | 53 | 65.618 | 47.212 | -7.338 | 1.00 28.33 | CPS1 |
| ATOM | 421 | ΝE | ARG | 53 | 66.937 | 47.751 | -7.675 | 1.00 29.58 | CPS1 |
| MOTA | 422 | cz | ARG | 53 | 67.976 | 46.986 | -7.980 | 1.00 29.37 | CPS1 |
| ATOM | 423 | NH1 | ARG | 53 | 67.821 | 45.670 | -7.978 | 1.00 29.23 | CPS1 |
| ATOM | 424 | NH2 | ARG | 53 | 69.153 | 47.525 | -8.299 | 1.00 26.48 | CPS1 |
| ATOM | 425 | C | ARG | 53 | 61.752 | 47.468 | -5.336 | 1.00 23.34 | CPS1 |
| ATOM | 426 | 0 | ARG | 53 | 61.921 | 48.237 | -4.389 | 1.00 22.79 | CPS1 |
| ATOM | 427 | N | PHE | 54 | 60.551 | 47.146 | -5.801 | 1.00 22.67 | CPS1 |
| ATOM | 428 | CA | PHE | 54 | 59.335 | 47.638 | -5.181 | 1.00 22.96 | CPS1 |
| ATOM | 429 | CB | PHE | 54 | 58.114 | 47.106 | -5.947 | 1.00 22.72 | CPS1 |
| ATOM | 430 | CG | PHE | 54 | 56.807 | 47.619 | -5.429 | 1.00 24.49 | CPS1 |
| ATOM | 431 | CD1 | PHE | 54 | 56.074 | 46.882 | -4.506 | 1.00 24.85 | CPS1 |
| ATOM | 432 | CD2 | PHE | 54 | 56.329 | 48.865 | -5.828 | 1.00 24.29 | CPS1 |
| MOTA | 433 | CE1 | PHE | 54 | 54.883 | 47.376 | -3.983 | 1.00 25.96 | CPS1 |
| ATOM | 434 | CE2 | PHE | 54 | 55.143 | 49.370 | -5.316 | 1.00 25.86 | CPS1 |
| ATOM | 435 | CZ | PHE | 54 | 54.414 | 48.624 | | 1.00 26.67 | CPS1 |
| ATOM | 436 | C | PHE | 54 | 59.285 | 47.177 | -3.724 | 1.00 22.66 | CPS1 |
| ATOM | 437 | 0 | PHE | 54 | 59.018 | 47.970 | | 1.00 21.27 | CPS1 |
| ATOM | 438 | N | ALA | 55 | 59.556 | 45.896 | | 1.00 20.95 | CPS1 |
| ATOM | 439 | CA | ALA | 55 | 59.524 | 45.349 | | 1.00 20.91 | CPS1 |
| ATOM | 440 | CB | ALA | 55 | 59.733 | 43.846 | | 1.00 20.44 | CPS1 |
| ATOM | 441 | C | ALA | 55 | 60.568 | 45.990 | | 1.00 20.32 | CPS1 |
| ATOM | 442 | ō | ALA | 55 | 60.288 | 46.295 | | 1.00 18.66 | CPS1 |
| ATOM | 443 | N | ALA | 56 | 61.779 | 46.172 | | 1.00 18.74 | CPS1 |
| ATOM | 444 | CA | ALA | 56 | 62.861 | 46.761 | | 1.00 19.35 | CPS1 |
| | 445 | CB | ALA | 56 | 64.180 | 46.698 | | 1.00 19.52 | CPS1 |
| ATOM | | | | | | | | 1.00 20.45 | CPS1 |
| MOTA | 446 | C | ALA | 56 | 62.543 | 48.201 | | 1.00 20.43 | CPS1 |
| ATOM | 447 | 0 | ALA | 56 53 | 62.773 | 48.617 | | 1.00 18.32 | CPS1 |
| MOTA | 448 | И | LYS | 57 | 62.015 | 48.969 | | | |
| MOTA | 449 | CA | LYS | 57 | 61.677 | 50.352 | | 1.00 19.87 | CPS1 |
| ATOM | 450 | CB | LYS | 57 | 61.427 | 51.107 | | 1.00 19.77 | CPS1 |
| ATOM | 451 | CG | LYS | 57 | 62.707 | 51.225 | | 1.00 20.64 | CPS1 |
| ATOM | 452 | CD | LYS | 57 | 62.533 | 52.055 | | 1.00 21.45 | CPS1 |
| ATOM | 453 | CE | LYS | 57 | 63.801 | 51.995 | | 1.00 22.31 | CPS1 |
| MOTA | 454 | NZ | LYS | 57 | 63.888 | 53.112 | | 1.00 22.70 | CPS1 |
| ATOM | 455 | C | LYS | 57 | 60.487 | 50.461 | -0.329 | 1.00 19.95 | CPS1 |

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| 3.000 | 450 | ^ | T 1/0 | | 60 450 | C1 7C2 | 0 575 | 1 00 00 70 | |
|-------|-----|-----|-------|----|--------|-------------|--------|------------|------|
| ATOM | 456 | 0 | LYS | 57 | 60.458 | 51.352 | 0.515 | 1.00 20.79 | CPS1 |
| ATOM | 457 | N | GLU | 58 | 59.513 | 49.561 | -0.463 | 1.00 19.28 | CPS1 |
| ATOM | 458 | CA | GLU | 58 | 58.358 | 49.567 | 0.436 | 1.00 21.04 | CPS1 |
| ATOM | 459 | CB | GLU | 58 | 57.324 | 48.516 | 0.013 | 1.00 22.82 | CPS1 |
| ATOM | 460 | CG | GLU | 58 | 56.428 | 48.907 | -1.170 | 1.00 28.45 | CPS1 |
| ATOM | 461 | CD | GLU | 58 | 55.586 | 50.145 | -0.886 | 1.00 31.31 | CPS1 |
| ATOM | 462 | OE1 | GLU | 58 | 55.244 | 50.371 | 0.295 | 1.00 33.36 | CPS1 |
| MOTA | 463 | OE2 | GLU | 58 | 55.253 | 50.886 | -1.840 | 1.00 34.15 | CPS1 |
| MOTA | 464 | C | GLU | 58 | 58.851 | 49.242 | 1.856 | 1.00 19.94 | CPS1 |
| MOTA | 465 | 0 | GLU | 58 | 58.456 | 49.899 | 2.818 | 1.00 19.84 | CPS1 |
| ATOM | 466 | N | ALA | 59 | 59.717 | 48.234 | 1.979 | 1.00 18.95 | CPS1 |
| ATOM | 467 | CA | ALA | 59 | 60.251 | 47.861 | 3.300 | 1.00 19.85 | CPS1 |
| ATOM | 468 | CB | ALA | 59 | 61.155 | 46.618 | 3.185 | 1.00 18.19 | CPS1 |
| ATOM | 469 | C | ALA | 59 | 61.044 | 49.037 | 3.881 | 1.00 20.46 | CPS1 |
| ATOM | 470 | 0 | ALA | 59 | 60.954 | 49.359 | 5.076 | 1.00 20.70 | CPS1 |
| | | | PHE | | | 49.691 | 3.042 | 1.00 19.23 | CPS1 |
| MOTA | 471 | N | | 60 | 61.831 | | | | |
| ATOM | 472 | CA | PHE | 60 | 62.606 | 50.824 | 3.538 | 1.00 19.91 | CPS1 |
| ATOM | 473 | CB | PHE | 60 | 63.500 | 51.407 | 2.440 | 1.00 20.97 | CPS1 |
| MOTA | 474 | CG | PHE | 60 | 64.280 | 52.613 | 2.893 | 1.00 21.48 | CPS1 |
| MOTA | 475 | CD1 | | 60 | 65.503 | 52.463 | 3.530 | 1.00 21.47 | CPS1 |
| ATOM | 476 | | PHE | 60 | 63.737 | 53.891 | 2.768 | 1.00 23.08 | CPS1 |
| MOTA | 477 | | PHE | 60 | 65.183 | 53.576 | 4.053 | 1.00 22.10 | CPS1 |
| MOTA | 478 | CE2 | PHE | 60 | 64.403 | 55.017 | 3.286 | 1.00 23.29 | CPS1 |
| ATOM | 479 | cz | PHE | 60 | 65.628 | 54.852 | 3.930 | 1.00 23.90 | CPS1 |
| ATOM | 480 | C | PHE | 60 | 61.673 | 51.919 | 4.047 | 1.00 20.74 | CPS1 |
| ATOM | 481 | 0 | PHE | 60 | 61.916 | 52.515 | 5.098 | 1.00 21.03 | CPS1 |
| MOTA | 482 | И | SER | 61 | 60.604 | 52.191 | 3.302 | 1.00 20.69 | CPS1 |
| MOTA | 483 | CA | SER | 61 | 59.669 | 53.237 | 3.702 | 1.00 21.92 | CPS1 |
| MOTA | 484 | CB | SER | 61 | 58.625 | 53.488 | 2.607 | 1.00 22.10 | CPS1 |
| MOTA | 485 | OG | SER | 61 | 57.716 | 52.406 | 2.499 | 1.00 23.85 | CPS1 |
| MOTA | 486 | C | SER | 61 | 58.967 | 52.917 | 5.020 | 1.00 22.52 | CPS1 |
| MOTA | 487 | 0 | SER | 61 | 58.574 | 53.824 | 5.760 | 1.00 23.57 | CPS1 |
| ATOM | 488 | N | LYS | 62 | 58.811 | 51.633 | 5.314 | 1.00 21.64 | CPS1 |
| MOTA | 489 | CA | LYS | 62 | 58.170 | 51.220 | 6.563 | 1.00 22.44 | CPS1 |
| MOTA | 490 | CB | LYS | 62 | 57.705 | 49.767 | 6.463 | 1.00 22.20 | CPS1 |
| MOTA | 491 | CG | LYS | 62 | 56.539 | 49.575 | 5.483 | 1.00 25.33 | CPS1 |
| MOTA | 492 | CD | LYS | 62 | 56.149 | 48.113 | 5.354 | 1.00 29.01 | CPS1 |
| MOTA | 493 | CE | LYS | 62 | 54.862 | 47.975 | 4.560 | 1.00 32.68 | CPS1 |
| ATOM | 494 | NZ | LYS | 62 | 54.355 | 46.585 | 4.526 | 1.00 36.07 | CPS1 |
| ATOM | 495 | C | LYS | 62 | 59.155 | 51.392 | 7.719 | 1.00 22.39 | CPS1 |
| MOTA | 496 | 0 | LYS | 62 | 58.782 | 51.841 | 8.806 | 1.00 21.87 | CPS1 |
| ATOM | 497 | N | ALA | 63 | 60.413 | 51.040 | 7.479 | 1.00 20.82 | CPS1 |
| MOTA | 498 | CA | ALA | 63 | 61.444 | 51.194 | 8.502 | 1.00 21.70 | CPS1 |
| MOTA | 499 | CB | ALA | 63 | 62.755 | 50.574 | 8.022 | 1.00 22.55 | CPS1 |
| MOTA | 500 | С | ALA | 63 | 61.633 | 52.688 | 8.786 | 1.00 23.41 | CPS1 |
| ATOM | 501 | 0 | ALA | 63 | 61.886 | 53.092 | 9.928 | 1.00 22.35 | CPS1 |
| ATOM | 502 | N | PHE | 64 | 61.498 | 53.498 | 7.737 | 1.00 23.23 | CPS1 |
| ATOM | 503 | CA | PHE | 64 | 61.638 | 54.946 | 7.838 | 1.00 25.59 | CPS1 |
| ATOM | 504 | CB | PHE | 64 | 61.638 | 55.559 | 6.430 | 1.00 27.30 | CPS1 |
| MOTA | 505 | CG | PHE | 64 | 62.121 | 56.979 | 6.381 | 1.00 30.46 | CPS1 |
| MOTA | 506 | | PHE | 64 | 63.464 | 57.279 | 6.593 | 1.00 31.49 | CPS1 |
| ATOM | 507 | | PHE | 64 | 61.237 | 58.015 | 6.107 | 1.00 29.70 | CPS1 |
| ATOM | 508 | | PHE | 64 | 63.920 | 58.596 | 6.528 | 1.00 33.53 | CPS1 |
| ATOM | 509 | | PHE | 64 | 61.681 | 59.333 | 6.039 | 1.00 31.57 | CPS1 |
| ATOM | 510 | CZ | PHE | 64 | 63.021 | 59.624 | | 1.00 32.65 | CPS1 |
| ATOM | 511 | C | PHE | 64 | 60.477 | 55.504 | | | CPS1 |
| ATOM | 512 | Ö | PHE | 64 | 60.564 | 56.613 | | | CPS1 |
| | | - | | | | | | | |

| ATOM | 513 | N | GLY | 65 | 59.388 | 54.735 | 8.751 | 1.00 27.22 | CPS1 |
|---------------|------------------|------------|-----|-----|-----------|--------|--------|------------|------|
| ATOM | 514 | CA | GLY | 65 | 58.229 | 55.102 | 9.554 | 1.00 28.06 | CPS1 |
| ATOM | 515 | C | GLY | 65 | 57.135 | 55.940 | 8.923 | 1.00 29.26 | CPS1 |
| ATOM | 516 | Ō | GLY | 65 | 56.143 | 56.260 | 9.577 | 1.00 29.04 | CPS1 |
| ATOM | 517 | N | THR | 66 | 57.299 | 56.279 | 7.650 | 1.00 29.45 | CPS1 |
| ATOM | 518 | CA | THR | 66 | 56.333 | 57.119 | 6.951 | 1.00 29.43 | |
| ATOM | 519 | CB | THR | 66 | 57.033 | 58.351 | | | CPS1 |
| | | | | | | | 6.391 | 1.00 30.19 | CPS1 |
| ATOM | 520 | OG1 | | 66 | 57.997 | 57.922 | 5.424 | 1.00 31.68 | CPS1 |
| ATOM | 521 | CG2 | THR | 66 | 57.751 | 59.114 | 7.489 | 1.00 31.63 | CPS1 |
| ATOM | 522 | C | THR | 66 | 55.640 | 56.453 | 5.764 | 1.00 30.61 | CPS1 |
| MOTA | 523 | 0 | THR | 66 | 54.548 | 56.862 | 5.365 | 1.00 30.50 | CPS1 |
| MOTA | 524 | N | GLY | 67 | 56.280 | 55.443 | 5.188 | 1.00 30.12 | CPS1 |
| MOTA | 525 | CA | GLY | 67 | 55.713 | 54.809 | 4.011 | 1.00 30.43 | CPS1 |
| ATOM | 526 | C | GLY | 67 | 56.020 | 55.750 | 2.852 | 1.00 31.44 | CPS1 |
| MOTA | 527 | 0 | GLY | 67 | 56.622 | 56.806 | 3.058 | 1.00 30.31 | CPS1 |
| MOTA | 528 | N | ILE | 68 | 55.626 | 55.383 | 1.639 | 1.00 31.40 | CPS1 |
| ATOM | 529 | CA | ILE | 68 | 55.886 | 56.239 | 0.486 | 1.00 32.28 | CPS1 |
| MOTA | 530 | CB | ILE | 68 | 55.869 | 55.429 | -0.844 | 1.00 31.80 | CPS1 |
| MOTA | 531 | CG2 | ILE | 68 | 56.083 | 56.375 | -2.048 | 1.00 32.06 | CPS1 |
| ATOM | 532 | CG1 | ILE | 68 | 56.975 | 54.364 | -0.826 | 1.00 29.99 | CPS1 |
| ATOM | 533 | CD1 | ILE | 68 | 58.391 | 54.924 | -0.821 | 1.00 29.70 | CPS1 |
| MOTA | 534 | C | ILE | 68 | 54.812 | 57.315 | 0.429 | 1.00 33.69 | CPS1 |
| MOTA | 535 | 0 | ILE | 68 | 53.623 | 57.028 | 0.556 | 1.00 34.51 | CPS1 |
| MOTA | 536 | N | GLY | 69 | 55.233 | 58.558 | 0.248 | 1.00 35.19 | CPS1 |
| ATOM | 537 | CA | GLY | 69 | 54.281 | 59.649 | 0.187 | 1.00 36.88 | CPS1 |
| ATOM | 538 | C | GLY | 69 | 54.989 | 60.985 | 0.167 | 1.00 37.34 | CPS1 |
| ATOM | 539 | 0 | GLY | 69 | 56.065 | 61.115 | -0.413 | 1.00 37.87 | CPS1 |
| ATOM | 540 | N | ALA | 70 | 54.394 | 61.977 | 0.821 | 1.00 38.19 | CPS1 |
| ATOM | 541 | CA | ALA | 70 | 54.964 | 63.314 | 0.866 | 1.00 38.33 | CPS1 |
| MOTA | 542 | CB | ALA | 70 | 54.010 | 64.252 | 1.609 | 1.00 39.53 | CPS1 |
| MOTA | 543 | C | ALA | 70 | 56.352 | 63.383 | 1.493 | 1.00 38.24 | CPS1 |
| ATOM | 544 | 0 | ALA | 70 | 57.188 | 64.171 | 1.067 | 1.00 39.11 | CPS1 |
| ATOM | 545 | N | GLN | 71 | 56.612 | 62.547 | 2.494 | 1.00 38.21 | CPS1 |
| ATOM | 546 | CA | GLN | 71 | 57.901 | 62.578 | 3.177 | 1.00 37.58 | CPS1 |
| ATOM | 547 | CB | GLN | 71 | 57.704 | 62.177 | 4.642 | 1.00 40.14 | CPS1 |
| MOTA | 548 | CG | GLN | 71 | 56.511 | 62.867 | 5.297 | 1.00 44.12 | CPS1 |
| | | | GLN | 71 | 56.276 | 62.410 | 6.724 | 1.00 45.82 | CPS1 |
| ATOM | 549 | CD | | 71 | 57.140 | 62.570 | 7.587 | 1.00 45.65 | CPS1 |
| ATOM | 550 | OE1 NE2 | | 71 | 55.101 | | 6.980 | 1.00 46.84 | CPS1 |
| ATOM | 551 | | | | | 61.838 | | | CPS1 |
| ATOM | 552 | C | GLN | 71 | 58.997 | 61.706 | 2.557 | 1.00 35.81 | CPS1 |
| ATOM | 553 | 0 | GLN | 71 | 60.175 | 61.854 | 2.885 | 1.00 35.04 | CPS1 |
| ATOM | 554 | N | LEU | 72 | 58.619 | 60.805 | 1.662 | 1.00 33.50 | |
| MOTA | 555 | CA | LEU | 72 | 59.602 | 59.917 | 1.053 | 1.00 31.98 | CPS1 |
| MOTA | 556 | CB | LEU | 72 | 59.899 | 58.762 | 2.010 | 1.00 30.93 | CPS1 |
| ATOM | 557 | CG | LEU | 72 | 60.905 | 57.699 | 1.561 | 1.00 30.26 | CPS1 |
| MOTA | 558 | | LEU | 72 | 62.311 | 58.276 | 1.592 | 1.00 31.32 | CPS1 |
| ATOM | 55 9 | | LEU | 72 | 60.801 | 56.483 | 2.490 | 1.00 29.64 | CPS1 |
| ATOM | 560 | C | LEU | 72 | 59.104 | 59.364 | -0.269 | 1.00 30.33 | CPS1 |
| MOTA | 561 | 0 | LEU | 72 | 58.025 | 58.794 | -0.333 | 1.00 30.73 | CPS1 |
| ATOM | 562 | N | SER | 73 | 59.907 | 59.526 | -1.315 | 1.00 30.09 | CPS1 |
| ATOM | 563 | CA | SER | 73 | 59.550 | 59.051 | -2.649 | 1.00 30.01 | CPS1 |
| ATOM | 564 | CB | SER | 73 | 59.795 | 60.161 | -3.679 | 1.00 30.79 | CPS1 |
| ATOM | 565 | OG | SER | 73 | 59.700 | 59.659 | -5.007 | 1.00 33.48 | CPS1 |
| MOTA | 566 | C | SER | 73 | 60.348 | 57.824 | -3.070 | 1.00 28.08 | CPS1 |
| MOTA | 567 | 0 | SER | 73 | 61.447 | 57.596 | -2.574 | 1.00 28.49 | CPS1 |
| MOTA | 568 | N | PHE | 74 | 59.792 | 57.032 | -3.985 | 1.00 28.86 | CPS1 |
| ATOM | 569 | CA | PHE | 74 | 60.512 | 55.869 | -4.502 | 1.00 28.18 | CPS1 |
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| MOTA | 570 | CB | PHE | 74 | 59.712 | 55.173 | -5.608 | 1.00 28.46 | CPS1 |
|------|-------------|-----|-----|------------|------------------|------------------|------------------|------------|--------------|
| MOTA | 571 | CG | PHE | 74 | 58.581 | 54.331 | -5.106 | 1.00 28.51 | CPS1 |
| MOTA | 572 | CD1 | PHE | 74 | 58.833 | 53.164 | -4.398 | 1.00 29.22 | CPS1 |
| MOTA | 573 | | PHE | 74 | 57.264 | 54.695 | -5.358 | 1.00 28.56 | CPS1 |
| MOTA | 574 | CE1 | PHE | 74 | 57.789 | 52.364 | -3.951 | 1.00 29.35 | CPS1 |
| ATOM | 575 | CE2 | PHE | 74 | 56.213 | 53.907 | -4.914 | 1.00 30.56 | CPS1 |
| ATOM | 576 | CZ | PHE | 74 | 56.479 | 52.734 | -4.209 | 1.00 28.99 | CPS1 |
| ATOM | 57 7 | С | PHE | 74 | 61.818 | 56.377 | -5.107 | 1.00 29.02 | CPS1 |
| ATOM | 578 | 0 | PHE | 74 | 62.846 | 55.697 | -5.076 | 1.00 28.52 | CPS1 |
| ATOM | 579 | N | GLN | 75 | 61.776 | 57.586 | -5.660 | 1.00 29.54 | CPS1 |
| ATOM | 580 | CA | GLN | 75 | 62.959 | 58.168 | -6.289 | 1.00 30.04 | CPS1 |
| ATOM | 581 | CB | GLN | 75 | 62.555 | 59.395 | -7.117 | 1.00 31.75 | CPS1 |
| ATOM | 582 | CG | GLN | 75 | 61.636 | 59.056 | -8.284 | 1.00 31.66 | CPS1 |
| ATOM | 583 | CD | GLN | 75 | 62.300 | 58.137 | -9.295 | 1.00 32.50 | CPS1 |
| ATOM | 584 | | GLN | 75 | 61.673 | 57.207 | -9.816 | 1.00 34.26 | CPS1 |
| MOTA | 585 | NE2 | | 75 | 63.571 | 58.396 | -9.584 | 1.00 30.64 | CPS1 |
| MOTA | 586 | С | GLN | 75 | 64.052 | 58.543 | -5.294 | 1.00 30.56 | CPS1 |
| MOTA | 587 | 0 | GLN | 75 | 65.205 | 58.768 | -5.681 | 1.00 29.97 | CPS1 |
| ATOM | 588 | N | ASP | 76 | 63.697 | 58.605 | -4.011 | 1.00 30.64 | CPS1 |
| ATOM | 589 | CA | ASP | 76 | 64.669 | 58.943 | -2.972 | 1.00 29.57 | CPS1 |
| ATOM | 590 | CB | ASP | 76 | 63.975 | 59.494 | -1.718 | 1.00 30.95 | CPS1 |
| ATOM | 591 | CG | ASP | 76 | 63.293 | 60.824 | -1.955 | 1.00 30.35 | CPS1 |
| ATOM | 592 | | ASP | 76 | 63.804 | 61.614 | -2.771 | 1.00 32.00 | CPS1 |
| ATOM | 593 | | ASP | 76 | 62.254 | 61.083 | -1.313 | 1.00 33.58 | CPS1 |
| ATOM | 594 | C | ASP | 76 | 65.472 | 57.720 | -2.546 | 1.00 32.57 | CPS1 |
| ATOM | 595 | 0 | ASP | 76 | 66.430 | 57.720 | -1.788 | 1.00 28.90 | CPS1 |
| ATOM | 596 | Ŋ | ILE | 77 | 65.085 | 56.551 | -3.038 | 1.00 27.41 | CPS1 |
| ATOM | 597 | CA | ILE | 7.7 7.7 | 65.752 | 55.318 | -2.644 | 1.00 27.41 | CPS1 |
| ATOM | 598 | CB | ILE | 77 | 64.750 | 54.372 | -1.947 | 1.00 25.25 | CPS1 |
| ATOM | 599 | CG2 | | 77 | 65.494 | 53.213 | -1.295 | 1.00 25.83 | CPS1 |
| | 600 | CG1 | | 77 | | 55.145 | -0.912 | 1.00 25.55 | CPS1 |
| ATOM | | | ILE | 77 | 63.927 62.613 | 54.455 | -0.547 | 1.00 25.71 | CPS1 |
| ATOM | 601 602 | CDI | ILE | 77 | 66.323 | 54.562 | -3.830 | 1.00 25.71 | CPS1 |
| ATOM | | | ILE | 77 | | | | 1.00 28.41 | CPS1 |
| ATOM | 603 | 0 | GLU | 78 | 65.633 | 54.355 | -4.819 -3.726 | 1.00 26.24 | CPS1 |
| ATOM | 604 | N | GLU | 78 | 67.573 | 54.134 53.359 | -4.800 | 1.00 26.24 | CPS1 |
| ATOM | 605 | CA | | | 68.179 | 54.197 | | 1.00 28.41 | CPS1 |
| MOTA | 606 | CB | GLU | 78 78 | 69.198 | 53.392 | -5.586 -6.661 | 1.00 27.49 | CPS1 |
| ATOM | 607 | CG | GLU | 78 70 | 69.942 | | | 1.00 34.35 | CPS1 |
| ATOM | 608 | CD | GLU | 78 70 | 70.711 | 54.265 54.887 | -7.657 | 1.00 34.33 | CPS1 |
| ATOM | 609 | OE1 | GLU | 78 78 | 70.059 | 54.328 | -8.526 -7.568 | 1.00 34.83 | CPS1 |
| ATOM | 610 | | | | 71.959 | | | 1.00 34.83 | |
| MOTA | 611 | C | GLU | 78 | 68.856 | 52.116 | -4.235 | | CPS1 CPS1 |
| ATOM | 612 | 0 | GLU | 78 | 69.581 | 52.183 | -3.244 | 1.00 26.47 | |
| ATOM | 613 | N | ILE | 79 | 68.595 | 50.976 | -4.863 | 1.00 26.08 | CPS1 CPS1 |
| MOTA | 614 | CA | ILE | 79 | 69.205 | 49.731 | -4.445 | 1.00 25.84 | |
| ATOM | 615 | CB | ILE | 79 | 68.192 | 48.545 | -4.459 | 1.00 25.79 | CPS1 |
| ATOM | 616 | | ILE | 79 | 68.942 | 47.221 | -4.467 | 1.00 25.99 | CPS1 |
| ATOM | 617 | | ILE | 79 | 67.282 | 48.595 | -3.224 | 1.00 28.30 | CPS1 |
| ATOM | 618 | | ILE | 79 | 66.246 | 49.685 | -3.247 | 1.00 25.92 | CPS1 |
| ATOM | 619 | C | ILE | 79 | 70.329 | 49.419 | -5.420 | 1.00 26.11 | CPS1 |
| ATOM | 620 | 0 | ILE | 79 | 70.186 | 49.598 | -6.633 | 1.00 24.92 | CPS1 |
| ATOM | 621 | N | ARG | 80 | 71.455 | 48.974 | -4.876 | 1.00 26.85 | CPS1 |
| ATOM | 622 | CA | ARG | 80 | 72.604 | 48.582 | -5.675 | 1.00 26.89 | CPS1 |
| ATOM | 623 | CB | ARG | 80 | 73.708 | 49.616 | -5.587 | 1.00 29.63 | CPS1 |
| MOTA | 624 | CG | ARG | 80 | 73.353 | 50.965 | -6.123 | 1.00 31.02 | CPS1 |
| ATOM | 625 | CD | ARG | 80 | 74.524 | 51.844 | -5.838 | 1.00 35.09 | CPS1 |
| ATOM | 626 | NE | ARG | 80 | 74.282 | 53.237 | -6.147 | 1.00 35.47 | CPS1 |

| ATOM | 627 | CZ | ARG | 80 | 75.084 | 54.205 | -5.736 | 1.00 33.96 | CPS1 |
|-------|-----|-----|-------|----|------------------|--------|--------|------------|------|
| ATOM | 628 | NH1 | ARG | 80 | 76.149 | 53.896 | -5.009 | 1.00 32.40 | CPS1 |
| MOTA | 629 | NH2 | ARG | 80 | 74.824 | 55.460 | -6.053 | 1.00 34.37 | CPS1 |
| MOTA | 630 | С | ARG | 80 | 73.130 | 47.294 | -5.090 | 1.00 27.91 | CPS1 |
| MOTA | 631 | 0 | ARG | 80 | 72.704 | 46.877 | -4.017 | 1.00 26.72 | CPS1 |
| MOTA | 632 | N | LYS | 81 | 74.061 | 46.662 | -5.794 | 1.00 28.40 | CPS1 |
| ATOM | 633 | CA | LYS | 81 | 74.671 | 45.436 | -5.301 | 1.00 29.29 | CPS1 |
| ATOM | 634 | CB | LYS | 81 | 74.395 | 44.275 | -6.260 | 1.00 31.32 | CPS1 |
| ATOM | 635 | CG | LYS | 81 | 72.962 | 43.773 | -6.177 | 1.00 34.37 | CPS1 |
| ATOM | 636 | CD | LYS | 81 | 72.745 | 42.490 | -6.965 | 1.00 38.80 | CPS1 |
| ATOM | 637 | CE | LYS | 81 | 71.388 | 41.887 | -6.623 | 1.00 41.39 | CPS1 |
| ATOM | 638 | NZ | LYS | 81 | 71.175 | 40.558 | -7.270 | 1.00 45.04 | CPS1 |
| ATOM | 639 | C | LYS | 81 | 76.159 | 45.688 | -5.173 | 1.00 29.85 | CPS1 |
| MOTA | 640 | ō | LYS | 81 | 76.754 | 46.332 | -6.039 | 1.00 29.65 | CPS1 |
| MOTA | 641 | N | ASP | 82 | 76.768 | 45.225 | -4.088 | 1.00 28.96 | CPS1 |
| MOTA | 642 | CA | ASP | 82 | 78.194 | 45.443 | -3.952 | 1.00 29.85 | CPS1 |
| ATOM | 643 | CB | ASP | 82 | 78.642 | 45.423 | -2.480 | 1.00 29.47 | CPS1 |
| ATOM | 644 | CG | ASP | 82 | 78.413 | 44.095 | -1.796 | 1.00 28.92 | CPS1 |
| ATOM | 645 | | ASP | 82 | 78.331 | 43.051 | -2.471 | 1.00 28.92 | CPS1 |
| ATOM | 646 | | ASP | 82 | 78.346 | 44.105 | | | |
| | | | | | | | -0.552 | 1.00 30.21 | CPS1 |
| ATOM | 647 | C | ASP | 82 | 78.918 78.281 | 44.388 | -4.773 | 1.00 30.66 | CPS1 |
| ATOM | 648 | 0 | ASP | 82 | | 43.626 | -5.496 | 1.00 29.93 | CPS1 |
| ATOM | 649 | N | GLN | 83 | 80.239 | 44.342 | -4.667 | 1.00 32.99 | CPS1 |
| ATOM | 650 | CA | GLN | 83 | 81.023 | 43.394 | -5.450 | 1.00 34.77 | CPS1 |
| ATOM | 651 | CB | GLN | 83 | 82.512 | 43.700 | -5.287 | 1.00 37.08 | CPS1 |
| ATOM | 652 | CG | GLN | 83 | 82.860 | 45.145 | -5.635 | 1.00 38.94 | CPS1 |
| MOTA | 653 | CD | GLN | 83 | 84.352 | 45.399 | -5.653 | 1.00 40.99 | CPS1 |
| MOTA | 654 | | GLN | 83 | 85.032 | 45.115 | -6.643 | 1.00 42.58 | CPS1 |
| MOTA | 655 | | GLN | 83 | 84.874 | 45.925 | -4.549 | 1.00 41.73 | CPS1 |
| ATOM | 656 | C | GLN | 83 | 80.746 | 41.924 | -5.151 | 1.00 35.50 | CPS1 |
| ATOM | 657 | 0 | GLN | 83 | 81.123 | 41.056 | -5.930 | 1.00 35.54 | CPS1 |
| ATOM | 658 | N | ASN | 84 | 80.094 | 41.640 | -4.027 | 1.00 36.07 | CPS1 |
| ATOM | 659 | CA | ASN | 84 | 79.757 | 40.258 | -3.684 | 1.00 35.57 | CPS1 |
| ATOM | 660 | CB | ASN | 84 | 79.863 | 40.014 | -2.178 | 1.00 37.57 | CPS1 |
| MOTA | 661 | CG | ASN | 84 | 81.284 | 39.960 | -1.700 | 1.00 39.82 | CPS1 |
| MOTA | 662 | | ASN | 84 | 82.116 | 39.250 | -2.270 | 1.00 41.25 | CPS1 |
| MOTA | 663 | | ASN | 84 | 81.577 | 40.702 | -0.639 | 1.00 40.86 | CPS1 |
| MOTA | 664 | C | ASN | 84 | 78.335 | 39.937 | -4.113 | 1.00 34.27 | CPS1 |
| MOTA | 665 | 0 | ASN | 84 | 77.856 | 38.824 | -3.899 | 1.00 34.98 | CPS1 |
| MOTA | 666 | N | GLY | 85 | 77.659 | 40.914 | -4.706 | 1.00 31.13 | CPS1 |
| MOTA | 667 | CA | GLY | 85 | 76.289 | 40.703 | -5.137 | 1.00 29.50 | CPS1 |
| ATOM | 668 | C | GLY | 85 | 75.274 | 41.002 | -4.040 | 1.00 27.83 | CPS1 |
| ATOM | 669 | 0 | GLY | 85 | 74.089 | 40.743 | -4.209 | 1.00 27.44 | CPS1 |
| ATOM | 670 | N | LYS | 86 | 75.737 | 41.548 | -2.919 | 1.00 26.25 | CPS1 |
| ATOM | 671 | CA | LYS | 86 | 74.858 | 41.888 | -1.797 | 1.00 25.96 | CPS1 |
| ATOM | 672 | CB | LYS | 86 | 75.664 | 41.946 | ~0.500 | 1.00 26.50 | CPS1 |
| ATOM | 673 | CG | LYS | 86 | 74.905 | 42.542 | 0.680 | 1.00 26.15 | CPS1 |
| ATOM | 674 | CD | LYS | 86 | 73.833 | 41.595 | 1.234 | 1.00 24.85 | CPS1 |
| ATOM | 675 | CE | LYS | 86 | 73.002 | 42.312 | 2.322 | 1.00 24.53 | CPS1 |
| MOTA | 676 | NZ | LYS | 86 | 72.000 | 41.403 | 2.973 | 1.00 23.95 | CPS1 |
| ATOM | 677 | C | LYS | 86 | 74.164 | 43.232 | -2.002 | 1.00 24.92 | CPS1 |
| MOTA | 678 | Ö | LYS | 86 | 74.812 | 44.253 | -2.223 | 1.00 25.51 | CPS1 |
| ATOM | 679 | N | PRO | 87 | 72.830 | 43.256 | -1.938 | 1.00 24.79 | CPS1 |
| ATOM | 680 | CD | PRO | 87 | 71.858 | 42.148 | -1.905 | 1.00 26.28 | CPS1 |
| ATOM | 681 | CA | PRO | 87 | 72.157 | 44.538 | -2.123 | 1.00 23.90 | CPS1 |
| ATOM | 682 | CB | PRO | 87 | 70.702 | 44.136 | -2.356 | 1.00 25.37 | CPS1 |
| ATOM | 683 | CG | PRO | 87 | 70.571 | 42.868 | -1.581 | 1.00 26.57 | CPS1 |
| A2011 | 000 | | - 200 | Ο, | ,0.5,1 | | 2.002 | | |

| MOTA | 684 | C | PRO | 87 | 72.300 | 45.486 | -0.933 | 1.00 24.14 | CPS1 |
|------|-----|-----|---------|----------|--------|--------|--------|------------|------|
| MOTA | 685 | 0 | PRO | 87 | 72.355 | 45.061 | 0.222 | 1.00 23.36 | CPS1 |
| ATOM | 686 | N | TYR | 88 | 72.383 | 46.775 | -1.223 | 1.00 23.09 | CPS1 |
| MOTA | 687 | CA | TYR | 88 | 72.456 | 47.775 | -0.170 | 1.00 22.80 | CPS1 |
| ATOM | 688 | CB | TYR | 88 | 73.903 | 48.132 | 0.169 | 1.00 23.97 | CPS1 |
| ATOM | 689 | CG | TYR | 88 | 74.662 | 48.796 | -0.948 | 1.00 23.15 | CPS1 |
| MOTA | 690 | CD1 | | 88 | 74.617 | 50.176 | -1.121 | 1.00 23.81 | CPS1 |
| ATOM | 691 | CE1 | TYR | 88 | 75.334 | 50.803 | -2.148 | 1.00 24.04 | CPS1 |
| ATOM | 692 | CD2 | TYR | 88 | 75.438 | 48.042 | -1.823 | 1.00 23.00 | CPS1 |
| MOTA | 693 | CE2 | TYR | 88 | 76.163 | 48.653 | -2.853 | 1.00 23.00 | CPS1 |
| ATOM | 694 | CZ | TYR | 88 | 76.105 | 50.031 | -3.007 | 1.00 24.59 | CPS1 |
| | | | | | | | | | |
| MOTA | 695 | OH | TYR | 88 | 76.807 | 50.635 | -4.029 | 1.00 23.69 | CPS1 |
| ATOM | 696 | C | TYR | 88 | 71.697 | 48.978 | -0.676 | 1.00 24.07 | CPS1 |
| ATOM | 697 | 0 | TYR | 88 | 71.492 | 49.131 | -1.882 | 1.00 24.63 | CPS1 |
| ATOM | 698 | N | ILE | 89 | 71.265 | 49.821 | 0.247 | 1.00 23.90 | CPS1 |
| MOTA | 699 | CA | ILE | 89 | 70.486 | 50.992 | -0.096 | 1.00 24.96 | CPS1 |
| ATOM | 700 | CB | ILE | 89 | 69.183 | 51.038 | 0.763 | 1.00 25.43 | CPS1 |
| ATOM | 701 | CG2 | | 89 | 68.580 | 52.445 | 0.773 | 1.00 23.76 | CPS1 |
| MOTA | 702 | CG1 | ILE | 89 | 68.179 | 50.007 | 0.237 | 1.00 25.76 | CPS1 |
| MOTA | 703 | CD1 | ILE | 89 | 66.920 | 49.857 | 1.102 | 1.00 25.48 | CPS1 |
| MOTA | 704 | C | ILE | 89 | 71.230 | 52.304 | 0.086 | 1.00 26.98 | CPS1 |
| ATOM | 705 | 0 | ILE | 89 | 72.018 | 52.470 | 1.020 | 1.00 27.02 | CPS1 |
| MOTA | 706 | N | ILE | 90 | 70.984 | 53.227 | -0.840 | 1.00 28.88 | CPS1 |
| ATOM | 707 | CA | ILE | 90 | 71.543 | 54.567 | -0.750 | 1.00 31.89 | CPS1 |
| ATOM | 708 | CB | ILE | 90 | 72.383 | 54.968 | -1.983 | 1.00 34.52 | CPS1 |
| MOTA | 709 | CG2 | ILE | 90 | 72.685 | 56.465 | -1.930 | 1.00 35.39 | CPS1 |
| ATOM | 710 | CG1 | ILE | 90 | 73.692 | 54.176 | -2.020 | 1.00 34.95 | CPS1 |
| ATOM | 711 | CD1 | ILE | 90 | 74.585 | 54.381 | -0.812 | 1.00 36.25 | CPS1 |
| MOTA | 712 | C | ILE | 90 | 70.299 | 55.433 | -0.715 | 1.00 32.42 | CPS1 |
| MOTA | 713 | 0 | ILE | 90 | 69.450 | 55.342 | -1.599 | 1.00 32.97 | CPS1 |
| ATOM | 714 | N | CYS | 91 | 70.165 | 56.246 | 0.320 | 1.00 32.73 | CPS1 |
| MOTA | 715 | CA | CYS | 91 | 69.002 | 57.106 | 0.433 | 1.00 34.96 | CPS1 |
| ATOM | 716 | CB | CYS | 91 | 68.008 | 56.543 | 1.463 | 1.00 32.49 | CPS1 |
| ATOM | 717 | SG | CYS | 91 | 66.523 | 57.557 | 1.657 | 1.00 29.59 | CPS1 |
| ATOM | 718 | C | CYS | 91 | 69.452 | 58.494 | 0.848 | 1.00 38.10 | CPS1 |
| MOTA | 719 | 0 | CYS | 91 | 70.079 | 58.666 | 1.893 | 1.00 40.46 | CPS1 |
| ATOM | 720 | N | THR | 92 | 69.124 | 59.476 | 0.014 | 1.00 42.14 | CPS1 |
| ATOM | 721 | CA | THR | 92 | 69.489 | 60.870 | 0.246 | 1.00 45.56 | CPS1 |
| ATOM | 722 | CB | THR | 92 | 68.964 | 61.772 | -0.898 | 1.00 46.93 | CPS1 |
| ATOM | 723 | OG1 | THR | 92 | 67.552 | 61.562 | -1.069 | 1.00 48.39 | CPS1 |
| ATOM | 724 | CG2 | THR | 92 | 69.686 | 61.454 | -2.205 | 1.00 47.93 | CPS1 |
| MOTA | 725 | С | THR | 92 | 69.001 | 61.457 | 1.571 | 1.00 46.35 | CPS1 |
| ATOM | 726 | O | THR | 92 | 69.345 | 62.592 | 1.901 | 1.00 47.51 | CPS1 |
| ATOM | 727 | N | LYS | 93 | 68.211 | 60.703 | 2.332 | 1.00 46.09 | CPS1 |
| ATOM | 728 | CA | LYS | 93 | 67.714 | 61.218 | 3.602 | 1.00 46.14 | CPS1 |
| ATOM | 729 | CB | LYS | 93 | 66.214 | 60.944 | 3.725 | 1.00 46.87 | CPS1 |
| MOTA | 730 | CG | LYS | 93 | 65.395 | 61.870 | 2.837 | 1.00 48.42 | CPS1 |
| ATOM | 731 | CD | LYS | 93 | 63.903 | 61.704 | 3.034 | 1.00 49.49 | CPS1 |
| ATOM | 732 | CE | LYS | 93 | 63.148 | 62.908 | 2.482 | 1.00 50.63 | CPS1 |
| ATOM | 733 | NZ | LYS | 93 | 63.471 | 63.177 | 1.054 | 1.00 52.22 | CPS1 |
| ATOM | 734 | C | LYS | 93 | 68.452 | 60.733 | 4.844 | 1.00 45.50 | CPS1 |
| ATOM | 735 | 0 | LYS | 93 | 68.167 | 61.182 | 5.954 | 1.00 45.52 | CPS1 |
| ATOM | 736 | N | LEU | 94 | 69.408 | 59.829 | 4.657 | 1.00 44.83 | CPS1 |
| ATOM | 737 | CA | LEU | 94 | 70.200 | 59.313 | 5.770 | 1.00 44.48 | CPS1 |
| ATOM | 738 | CB | LEU | 94 | 69.376 | 58.330 | 6.611 | 1.00 44.44 | CPS1 |
| ATOM | 739 | CG | LEU | 94 94 | 68.488 | 57.283 | 5.928 | 1.00 44.15 | CPS1 |
| | 740 | | LEU | 94 | 69.258 | 56.498 | 4.886 | 1.00 42.30 | CPS1 |
| ATOM | 740 | CDT | ب دند . | 24 | 07.430 | 30.470 | 1.000 | | |

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| MOTA | 741 | CD2 | T.FTT | 94 | 67.934 | 56.361 | 6.997 | 1.00 43.28 | CDC1 |
|------|-----|-----|-------|-----|--------------|--------|-------|---------------------------------------|------|
| ATOM | 742 | C | LEU | 94 | 71.486 | 58.641 | 5.307 | 1.00 44.30 | CPS1 |
| | | | | | | | | | CPS1 |
| ATOM | 743 | 0 | LEU | 94 | 71.692 | 58.432 | 4.111 | 1.00 44.84 | CPS1 |
| MOTA | 744 | N | SER | 95 | 72.353 | 58.308 | 6.257 | 1.00 43.56 | CPS1 |
| ATOM | 745 | CA | SER | 95 | 73.612 | 57.655 | 5.934 | 1.00 44.17 | CPS1 |
| ATOM | 746 | CB | SER | 95 | 74.583 | 57.748 | 7.107 | 1.00 44.85 | CPS1 |
| MOTA | 747 | OG | SER | 95 | 75.803 | 57.098 | 6.784 | 1.00 47.82 | CPS1 |
| MOTA | 748 | C | SER | 95 | 73.408 | 56.184 | 5.577 | 1.00 43.59 | CPS1 |
| ATOM | 749 | 0 | SER | 95 | 72.676 | 55.462 | 6.258 | 1.00 43.06 | CPS1 |
| MOTA | 750 | N | PRO | 96 | 74.065 | 55.720 | 4.503 | 1.00 42.46 | CPS1 |
| ATOM | 751 | CD | PRO | 96 | 75.025 | 56.444 | 3.650 | 1.00 42.90 | CPS1 |
| ATOM | 752 | CA | PRO | 96 | 73.939 | 54.325 | 4.079 | 1.00 41.30 | CPS1 |
| ATOM | 753 | CB | PRO | 96 | 74.757 | 54.286 | 2.788 | 1.00 42.08 | CPS1 |
| ATOM | 754 | CG | PRO | 96 | 75.821 | 55.316 | 3.045 | 1.00 42.41 | CPS1 |
| | 755 | C | PRO | 96 | | | 5.153 | · · · · · · · · · · · · · · · · · · · | |
| ATOM | | | | | 74.473 | 53.379 | | 1.00 39.30 | CPS1 |
| ATOM | 756 | 0 | PRO | 96 | 74.098 | 52.210 | 5.206 | 1.00 38.17 | CPS1 |
| MOTA | 757 | И | ALA | 97 | 75.348 | 53.901 | 6.008 | 1.00 37.86 | CPS1 |
| ATOM | 758 | CA | ALA | 97 | 75.929 | 53.117 | 7.095 | 1.00 36.05 | CPS1 |
| MOTA | 759 | CB | ALA | 97 | 76.982 | 53.940 | 7.819 | 1.00 37.73 | CPS1 |
| MOTA | 760 | C | ALA | 97 | 74.857 | 52.681 | 8.090 | 1.00 35.10 | CPS1 |
| ATOM | 761 | 0 | ALA | 97 | 74.992 | 51.662 | 8.770 | 1.00 35.38 | CPS1 |
| MOTA | 762 | N | ALA | 98 | 73.789 | 53.460 | 8.173 | 1.00 33.38 | CPS1 |
| MOTA | 763 | CA | ALA | 98 | 72.717 | 53.160 | 9.107 | 1.00 31.76 | CPS1 |
| ATOM | 764 | CB | ALA | 98 | 72.057 | 54.454 | 9.546 | 1.00 33.83 | CPS1 |
| ATOM | 765 | С | ALA | 98 | 71.657 | 52.220 | 8.537 | 1.00 30.24 | CPS1 |
| ATOM | 766 | 0 | ALA | 98 | 70.734 | 51.849 | 9.255 | 1.00 31.14 | CPS1 |
| ATOM | 767 | N | VAL | 99 | 71.796 | 51.831 | 7.269 | 1.00 26.77 | CPS1 |
| ATOM | 768 | CA | VAL | 99 | 70.803 | 50.980 | 6.607 | 1.00 25.25 | CPS1 |
| ATOM | 769 | CB | VAL | 99 | 70.258 | 51.695 | 5.331 | 1.00 24.54 | CPS1 |
| | 770 | | VAL | 99 | 69.091 | 50.920 | 4.731 | 1.00 24.54 | CPS1 |
| MOTA | | | | | | | | | CPS1 |
| ATOM | 771 | | VAL | 99 | 69.829 | 53.107 | 5.676 | 1.00 26.14 | |
| ATOM | 772 | C | VAL | 99 | 71.272 | 49.576 | 6.207 | 1.00 23.74 | CPS1 |
| MOTA | 773 | 0 | VAL | 99 | 72.390 | 49.393 | 5.720 | 1.00 23.55 | CPS1 |
| MOTA | 774 | И | HIS | 100 | 70.395 | 48.595 | 6.422 | 1.00 22.48 | CPS1 |
| ATOM | 775 | CA | HIS | 100 | 70.640 | 47.195 | 6.075 | 1.00 21.75 | CPS1 |
| MOTA | 776 | CB | HIS | 100 | 70.873 | 46.360 | 7.334 | 1.00 23.99 | CPS1 |
| ATOM | 777 | CG | HIS | 100 | 72.020 | 46.846 | 8.160 | 1.00 27.42 | CPS1 |
| ATOM | 778 | CD2 | HIS | 100 | 72.060 | 47.696 | 9.212 | 1.00 28.79 | CPS1 |
| MOTA | 779 | NDl | HIS | 100 | 73.329 | 46.542 | 7.859 | 1.00 28.14 | CPS1 |
| ATOM | 780 | CE1 | HIS | 100 | 74.128 | 47.190 | 8.689 | 1.00 30.71 | CPS1 |
| ATOM | 781 | NE2 | HIS | 100 | 73.383 | 47.898 | 9.519 | 1.00 30.58 | CPS1 |
| ATOM | 782 | C | HIS | 100 | 69.394 | 46.686 | 5.357 | 1.00 20.99 | CPS1 |
| MOTA | 783 | 0 | HIS | 100 | 68.270 | 47.007 | 5.752 | 1.00 20.00 | CPS1 |
| ATOM | 784 | N | VAL | 101 | 69.593 | 45.893 | 4.312 | 1.00 20.41 | CPS1 |
| ATOM | 785 | CA | VAL | 101 | 68.473 | 45.357 | 3.551 | 1.00 20.21 | CPS1 |
| MOTA | 786 | CB | VAL | 101 | 68.181 | 46.244 | 2.290 | 1.00 20.23 | CPS1 |
| | | | | | | | 1.344 | 1.00 22.43 | CPS1 |
| ATOM | 787 | | VAL | 101 | 69.391 | 46.245 | | 1.00 21.20 | CPS1 |
| ATOM | 788 | | VAL | 101 | 66.958 | 45.723 | 1.553 | | |
| MOTA | 789 | С | VAL | 101 | 68.761 | 43.939 | 3.084 | 1.00 20.38 | CPS1 |
| ATOM | 790 | 0 | VAL | 101 | 69.920 | 43.527 | 2.986 | 1.00 19.26 | CPS1 |
| ATOM | 791 | N | SER | 102 | 67.702 | 43.167 | 2.835 | 1.00 19.19 | CPS1 |
| MOTA | 792 | CA | SER | 102 | 67.867 | 41.833 | 2.280 | 1.00 19.46 | CPS1 |
| ATOM | 793 | CB | SER | 102 | 67.884 | 40.742 | 3.345 | 1.00 18.79 | CPS1 |
| ATOM | 794 | OG | SER | 102 | 68.068 | 39.478 | 2.720 | 1.00 18.64 | CPS1 |
| MOTA | 795 | С | SER | 102 | 66.677 | 41.638 | 1.358 | 1.00 20.37 | CPS1 |
| ATOM | 796 | 0 | SER | 102 | 65.581 | 42.095 | 1.658 | 1.00 20.10 | CPS1 |
| ATOM | 797 | N | ILE | 103 | 66.902 | 40.964 | 0.236 | 1.00 19.92 | CPS1 |
| | | - | | | - | | | | |

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| ATOM | 798 | CA | ILE | 103 | 65.847 | 40.737 | -0.744 | 1.00 19.71 | CPS1 |
|------|-----|-----|-----|-----|------------------|--------|------------------|------------|------|
| ATOM | 799 | CB | ILE | 103 | 66.122 | 41.550 | -2.033 | 1.00 19.02 | CPS1 |
| ATOM | 800 | CG2 | ILE | 103 | 64.988 | 41.337 | -3.054 | 1.00 19.50 | CPS1 |
| ATOM | 801 | | ILE | 103 | 66.234 | 43.031 | -1.682 | 1.00 18.90 | CPS1 |
| ATOM | 802 | CD1 | | 103 | 66.767 | 43.904 | -2.828 | 1.00 19.01 | CPS1 |
| ATOM | 803 | C | ILE | 103 | 65.804 | 39.265 | -1.090 | 1.00 20.30 | CPS1 |
| ATOM | 804 | 0 | ILE | 103 | 66.847 | 38.620 | -1.164 | 1.00 20.97 | CPS1 |
| ATOM | 805 | N | THR | 104 | 64.603 | 38.729 | -1.287 | 1.00 20.48 | CPS1 |
| ATOM | 806 | CA | THR | 104 | 64.468 | 37.316 | | | |
| ATOM | 807 | CB | THR | 104 | | 36.462 | -1.623 -0.350 | 1.00 20.34 | CPS1 |
| | | | | | 64.172 | | | 1.00 21.86 | CPS1 |
| ATOM | 808 | OG1 | THR | 104 | 64.222 | 35.065 | -0.671 | 1.00 21.77 | CPS1 |
| ATOM | 809 | CG2 | THR | 104 | 62.804 | 36.795 | 0.213 | 1.00 20.65 | CPS1 |
| ATOM | 810 | C | THR | 104 | 63.346 | 37.139 | -2.642 | 1.00 21.68 | CPS1 |
| ATOM | 811 | 0 | THR | 104 | 62.501 | 38.018 | -2.813 | 1.00 20.50 | CPS1 |
| ATOM | 812 | N | HIS | 105 | 63.345 | 36.003 | -3.325 | 1.00 22.11 | CPS1 |
| MOTA | 813 | CA | HIS | 105 | 62.323 | 35.728 | -4.331 | 1.00 24.82 | CPS1 |
| MOTA | 814 | CB | HIS | 105 | 62.884 | 35.948 | -5.747 | 1.00 27.53 | CPS1 |
| MOTA | 815 | CG | HIS | 105 | 63.383 | 37.335 | -6.020 | 1.00 32.22 | CPS1 |
| MOTA | 816 | CD2 | HIS | 105 | 64.585 | 37.915 | -5.782 | 1.00 34.13 | CPS1 |
| ATOM | 817 | ND1 | HIS | 105 | 62.615 | 38.292 | -6.648 | 1.00 36.59 | CPS1 |
| ATOM | 818 | CE1 | HIS | 105 | 63.322 | 39.402 | -6.786 | 1.00 35.80 | CPS1 |
| ATOM | 819 | NE2 | HIS | 105 | 64.521 | 39.199 | -6.271 | 1.00 35.22 | CPS1 |
| ATOM | 820 | C | HIS | 105 | 61.863 | 34.268 | -4.280 | 1.00 24.66 | CPS1 |
| ATOM | 821 | 0 | HIS | 105 | 62.570 | 33.400 | -3.766 | 1.00 23.89 | CPS1 |
| ATOM | 822 | N | THR | 106 | 60.667 | 34.027 | -4.811 | 1.00 24.24 | CPS1 |
| ATOM | 823 | CA | THR | 106 | 60.127 | 32.677 | -5.003 | 1.00 24.46 | CPS1 |
| ATOM | 824 | CB | THR | 106 | 59.008 | 32.271 | -4.019 | 1.00 25.81 | CPS1 |
| ATOM | 825 | OG1 | | 106 | 57.840 | 33.073 | -4.253 | 1.00 25.01 | CPS1 |
| MOTA | 826 | CG2 | THR | 106 | 59.483 | 32.419 | -2.570 | 1.00 24.51 | CPS1 |
| ATOM | 827 | C | THR | 106 | 59.500 | 32.820 | -6.388 | 1.00 25.67 | CPS1 |
| MOTA | 828 | 0 | THR | 106 | 59.496 | 33.915 | -6.953 | 1.00 25.60 | CPS1 |
| MOTA | 829 | N | ALA | 107 | 58.962 | 31.740 | -6.939 | 1.00 25.39 | CPS1 |
| MOTA | 830 | CA | ALA | 107 | 58.355 | 31.824 | -8.262 | 1.00 25.43 | CPS1 |
| ATOM | 831 | CB | ALA | 107 | 57.743 | 30.463 | -8.637 | 1.00 25.15 | CPS1 |
| ATOM | 832 | C | ALA | 107 | 57.288 | 32.918 | -8.363 | 1.00 25.95 | CPS1 |
| ATOM | 833 | 0 | ALA | 107 | 57.233 | 33.660 | -9.353 | 1.00 25.81 | CPS1 |
| ATOM | 834 | N | GLU | 108 | 56.452 | 33.035 | -7.335 | 1.00 24.82 | CPS1 |
| ATOM | 835 | CA | GLU | 108 | 55.356 | 34.007 | -7.367 | 1.00 25.17 | CPS1 |
| | | | GLU | | 54.043 | | -7.008 | 1.00 23.17 | CPS1 |
| ATOM | 836 | CB | | 108 | | 33.295 | | 1.00 27.79 | CPS1 |
| ATOM | 837 | CG | GLU | 108 | 53.688 52.404 | 32.198 | -8.005 | | CPS1 |
| MOTA | 838 | CD | GLU | 108 | | 31.450 | -7.675 | 1.00 39.77 | CPS1 |
| MOTA | 839 | OE1 | | 108 | 52.146 | 30.431 | -8.355 | 1.00 43.18 | CPS1 |
| MOTA | 840 | | GLU | 108 | 51.652 | 31.864 | -6.758 | 1.00 42.25 | |
| MOTA | 841 | C | GLU | 108 | 55.486 | 35.267 | -6.507 | 1.00 24.23 | CPS1 |
| ATOM | 842 | 0 | GLU | 108 | 54.654 | 36.178 | -6.615 | 1.00 22.93 | CPS1 |
| ATOM | 843 | N | TYR | 109 | 56.518 | 35.330 | -5.669 | 1.00 21.86 | CPS1 |
| MOTA | 844 | CA | TYR | 109 | 56.678 | 36.480 | -4.788 | 1.00 21.64 | CPS1 |
| MOTA | 845 | CB | TYR | 109 | 56.320 | 36.077 | -3.352 | 1.00 22.31 | CPS1 |
| ATOM | 846 | CG | TYR | 109 | 54.889 | 35.632 | -3.180 | 1.00 23.87 | CPS1 |
| MOTA | 847 | | TYR | 109 | 53.868 | 36.562 | -2.999 | 1.00 23.05 | CPS1 |
| MOTA | 848 | | TYR | 109 | 52.546 | 36.164 | -2.894 | 1.00 24.80 | CPS1 |
| ATOM | 849 | CD2 | TYR | 109 | 54.550 | 34.283 | -3.253 | 1.00 24.86 | CPS1 |
| MOTA | 850 | CE2 | TYR | 109 | 53.226 | 33.872 | -3.154 | 1.00 27.10 | CPS1 |
| MOTA | 851 | CZ | TYR | 109 | 52.233 | 34.818 | -2.977 | 1.00 24.92 | CPS1 |
| ATOM | 852 | OH | TYR | 109 | 50.924 | 34.420 | -2.916 | 1.00 25.87 | CPS1 |
| ATOM | 853 | С | TYR | 109 | 58.066 | 37.100 | -4.741 | 1.00 21.01 | CPS1 |
| ATOM | 854 | 0 | TYR | 109 | 59.063 | 36.476 | -5.091 | 1.00 21.94 | CPS1 |
| | | _ | | | -2 | , • | | | |

| ATOM | 855 | N | ALA | 110 | 58.097 | 20 247 | -4.292 | 1 00 00 01 | 0701 |
|------|-------------|-----|-----|-----|--------|--------|--------|------------|------|
| | | | | | | 38.347 | | 1.00 20.81 | CPS1 |
| MOTA | 856 | CA | ALA | 110 | 59.344 | 39.074 | -4.057 | 1.00 20.89 | CPS1 |
| ATOM | 85 7 | CB | ALA | 110 | 59.483 | 40.256 | -5.013 | 1.00 21.11 | CPS1 |
| MOTA | 858 | C | ALA | 110 | 59.155 | 39.574 | -2.617 | 1.00 19.96 | CPS1 |
| MOTA | 859 | 0 | ALA | 110 | 58.043 | 39.941 | -2.238 | 1.00 21.37 | CPS1 |
| ATOM | 860 | N | ALA | 111 | 60.209 | 39.576 | -1.805 | 1.00 18.57 | CPS1 |
| ATOM | 861 | CA | ALA | 111 | 60.074 | 40.062 | -0.435 | 1.00 17.40 | CPS1 |
| | | | ALA | | | | | | |
| ATOM | 862 | CB | | 111 | 59.780 | 38.896 | 0.509 | 1.00 16.67 | CPS1 |
| MOTA | 863 | С | ALA | 111 | 61.362 | 40.756 | -0.023 | 1.00 17.97 | CPS1 |
| ATOM | 864 | 0 | ALA | 111 | 62.411 | 40.476 | -0.580 | 1.00 17.28 | CPS1 |
| ATOM | 865 | N | ALA | 112 | 61.275 | 41.676 | 0.931 | 1.00 16.46 | CPS1 |
| MOTA | 866 | CA | ALA | 112 | 62.458 | 42.374 | 1.394 | 1.00 17.56 | CPS1 |
| ATOM | 867 | CB | ALA | 112 | 62.786 | 43.553 | 0.444 | 1.00 17.14 | CPS1 |
| MOTA | 868 | С | ALA | 112 | 62.263 | 42.880 | 2.809 | 1.00 16.81 | CPS1 |
| ATOM | 869 | ō | ALA | 112 | 61.143 | 43.042 | 3.270 | 1.00 17.67 | CPS1 |
| ATOM | 870 | N | GLN | 113 | 63.361 | 43.106 | 3.514 | 1.00 17.77 | CPS1 |
| | | | | | | | | | |
| MOTA | 871 | CA | GLN | 113 | 63.267 | 43.639 | 4.863 | 1.00 17.30 | CPS1 |
| ATOM | 872 | CB | GLN | 113 | 63.469 | 42.554 | 5.929 | 1.00 18.78 | CPS1 |
| MOTA | 873 | CG | GLN | 113 | 64.842 | 41.925 | 5.912 | 1.00 22.22 | CPS1 |
| MOTA | 874 | CD | GLN | 113 | 65.029 | 40.878 | 6.990 | 1.00 26.02 | CPS1 |
| ATOM | 875 | OE1 | GLN | 113 | 66.130 | 40.366 | 7.182 | 1.00 29.00 | CPS1 |
| MOTA | 876 | NE2 | GLN | 113 | 63.950 | 40.541 | 7.688 | 1.00 28.62 | CPS1 |
| ATOM | 877 | С | GLN | 113 | 64.370 | 44.658 | 4.985 | 1.00 18.39 | CPS1 |
| MOTA | 878 | ō | GLN | 113 | 65.410 | 44.550 | 4.338 | 1.00 19.07 | CPS1 |
| ATOM | 879 | N | VAL | 114 | 64.142 | 45.639 | 5.836 | 1.00 18.02 | CPS1 |
| | | | | | | 46.675 | 6.042 | 1.00 17.24 | CPS1 |
| ATOM | 880 | CA | VAL | 114 | 65.128 | | | | |
| MOTA | 881 | CB | VAL | 114 | 64.702 | 47.987 | 5.317 | 1.00 17.08 | CPS1 |
| ATOM | 882 | | VAL | 114 | 65.511 | 49.194 | 5.863 | 1.00 16.82 | CPS1 |
| ATOM | 883 | | VAL | 114 | 64.897 | 47.837 | 3.810 | 1.00 15.69 | CPS1 |
| MOTA | 884 | C | VAL | 114 | 65.223 | 46.962 | 7.526 | 1.00 18.35 | CPS1 |
| ATOM | 885 | 0 | VAL | 114 | 64.228 | 46.862 | 8.260 | 1.00 17.93 | CPS1 |
| MOTA | 886 | N | VAL | 115 | 66.429 | 47.280 | 7.973 | 1.00 19.07 | CPS1 |
| MOTA | 887 | CA | VAL | 115 | 66.622 | 47.702 | 9.351 | 1.00 20.05 | CPS1 |
| ATOM | 888 | CB | VAL | 115 | 67.435 | 46.698 | 10.193 | 1.00 21.79 | CPS1 |
| MOTA | 889 | | VAL | 115 | 67.695 | 47.297 | 11.582 | 1.00 24.02 | CPS1 |
| ATOM | 890 | CG2 | | 115 | 66.680 | 45.387 | 10.322 | 1.00 21.49 | CPS1 |
| | | | VAL | | | 49.003 | 9.266 | 1.00 20.53 | CPS1 |
| ATOM | 891 | C | | 115 | 67.411 | | | | CPS1 |
| MOTA | 892 | 0 | VAL | 115 | 68.416 | 49.077 | 8.552 | 1.00 19.46 | |
| ATOM | 893 | N | ILE | 116 | 66.921 | 50.038 | 9.943 | 1.00 22.12 | CPS1 |
| MOTA | 894 | CA | ILE | 116 | 67.620 | 51.321 | 9.987 | 1.00 22.75 | CPS1 |
| ATOM | 895 | CB | ILE | 116 | 66.694 | 52.492 | 9.629 | 1.00 22.88 | CPS1 |
| ATOM | 896 | CG2 | ILE | 116 | 67.430 | 53.825 | 9.850 | 1.00 23.51 | CPS1 |
| MOTA | 897 | CG1 | ILE | 116 | 66.232 | 52.353 | 8.172 | 1.00 22.44 | CPS1 |
| ATOM | 898 | CD1 | ILE | 116 | 65.208 | 53.382 | 7.742 | 1.00 20.81 | CPS1 |
| ATOM | 899 | C | ILE | 116 | 68.090 | 51.495 | 11.430 | 1.00 25.25 | CPS1 |
| ATOM | 900 | o | ILE | 116 | 67.312 | 51.296 | 12.363 | 1.00 22.08 | CPS1 |
| | | | | | | 51.845 | 11.610 | 1.00 28.24 | CPS1 |
| ATOM | 901 | N | GLU | 117 | 69.362 | | | | |
| MOTA | 902 | CA | GLU | 117 | 69.923 | 52.041 | 12.944 | 1.00 33.38 | CPS1 |
| ATOM | 903 | CB | GLU | 117 | 71.297 | 51.384 | 13.074 | 1.00 34.32 | CPS1 |
| MOTA | 904 | CG | GLU | 117 | 71.376 | 49.888 | 12.878 | 1.00 36.79 | CPS1 |
| ATOM | 905 | CD | GLU | 117 | 72.808 | 49.388 | 13.006 | 1.00 38.57 | CPS1 |
| ATOM | 906 | OE1 | GLU | 117 | 73.266 | 49.163 | 14.144 | 1.00 40.54 | CPS1 |
| ATOM | 907 | | GLU | 117 | 73.489 | 49.243 | 11.971 | 1.00 40.35 | CPS1 |
| ATOM | 908 | C | GLU | 117 | 70.119 | 53.524 | 13.216 | 1.00 36.51 | CPS1 |
| ATOM | 909 | Ö | GLU | 117 | 70.269 | 54.317 | 12.289 | 1.00 36.14 | CPS1 |
| | | | | | | 53.890 | 14.493 | 1.00 40.58 | CPS1 |
| ATOM | 910 | N | ARG | 118 | 70.120 | | | | CPS1 |
| ATOM | 911 | CA | ARG | 118 | 70.358 | 55.275 | 14.884 | 1.00 45.79 | CPSI |

| MOTA | 912 | CB | ARG | 118 | 69.712 | 55.600 | 16.235 | 1.00 46.59 | CPS1 |
|------|-------------|-----|-----|-----|--------|--------|--------|------------|------|
| ATOM | 913 | CG | ARG | 118 | 68.229 | 55.336 | 16.356 | 1.00 49.65 | CPS1 |
| ATOM | 914 | CD | ARG | 118 | 67.792 | 55.527 | 17.809 | 1.00 52.26 | CPS1 |
| MOTA | 915 | NE | ARG | 118 | 66.418 | 55.092 | 18.046 | 1.00 54.79 | CPS1 |
| ATOM | 916 | CZ | ARG | 118 | 65.337 | 55.786 | 17.702 | 1.00 55.39 | CPS1 |
| ATOM | 917 | NH1 | | 118 | 64.131 | 55.299 | 17.956 | 1.00 56.47 | CPS1 |
| | | | | | | | | | |
| MOTA | 918 | NH2 | | 118 | 65.458 | 56.972 | 17.120 | 1.00 56.32 | CPS1 |
| MOTA | 919 | C | ARG | 118 | 71.868 | 55.331 | 15.069 | 1.00 48.09 | CPS1 |
| MOTA | 920 | 0 | ARG | 118 | 72.435 | 54.481 | 15.755 | 1.00 49.38 | CPS1 |
| MOTA | 921 | N | LEU | 119 | 72:529 | 56.308 | 14.462 | 1.00 50.93 | CPS1 |
| ATOM | 922 | CA | LEU | 119 | 73.973 | 56.418 | 14.631 | 1.00 53.26 | CPS1 |
| ATOM | 923 | CB | LEU | 119 | 74.651 | 56.655 | 13.277 | 1.00 53.81 | CPS1 |
| MOTA | 924 | CG | LEU | 119 | 74.474 | 55.541 | 12.239 | 1.00 54.33 | CPS1 |
| | | | | | | | | | |
| ATOM | 925 | CD1 | | 119 | 75.203 | 55.906 | 10.953 | 1.00 54.92 | CPS1 |
| ATOM | 926 | CD2 | | 119 | 75.006 | 54.234 | 12.801 | 1.00 54.83 | CPS1 |
| MOTA | 927 | С | LEU | 119 | 74.286 | 57.568 | 15.591 | 1.00 54.40 | CPS1 |
| MOTA | 928 | OT1 | LEU | 119 | 74.613 | 57.278 | 16.765 | 1.00 55.09 | CPS1 |
| ATOM | 929 | OT2 | LEU | 119 | 74.177 | 58.740 | 15.166 | 1.00 55.10 | CPS1 |
| ATOM | 930 | С | GLY | 0 | 77.740 | 47.623 | 17.259 | 1.00 45.52 | CPS2 |
| MOTA | 931 | 0 | GLY | ٥ | 78.476 | 48.184 | 16.444 | 1.00 47.54 | CPS2 |
| ATOM | 932 | N | GLY | ٥ | 79.569 | 47.872 | 18.959 | 1.00 47.48 | CPS2 |
| ATOM | | | GLY | D | 78.237 | 47.280 | 18.650 | 1.00 47.48 | CPS2 |
| | 933 | CA | | | | | | | |
| MOTA | 934 | N | GLY | 1 | 76.484 | 47.284 | 16.983 | 1.00 43.42 | CPS2 |
| ATOM | 935 | CA | GLY | 1 | 75.916 | 47.570 | 15.679 | 1.00 38.90 | CPS2 |
| ATOM | 936 | С | GLY | 1 | 75.631 | 46.308 | 14.888 | 1.00 35.36 | CPS2 |
| MOTA | 937 | 0 | GLY | 1 | 76.138 | 45.233 | 15.198 | 1.00 35.52 | CPS2 |
| MOTA | 938 | N | ILE | 2 | 74.818 | 46.451 | 13.853 | 1.00 32.81 | CPS2 |
| ATOM | 939 | CA | ILE | 2 | 74.444 | 45.331 | 12.997 | 1.00 30.92 | CPS2 |
| ATOM | 940 | CB | ILE | 2 | 73.034 | 45.554 | 12.419 | 1.00 30.17 | CPS2 |
| ATOM | 941 | CG2 | | 2 | 72.715 | 44.495 | 11.369 | 1.00 28.15 | CPS2 |
| | | | | | | | | | CPS2 |
| ATOM | 942 | | ILE | 2 | 72.019 | 45.547 | 13.564 | 1.00 30.04 | |
| MOTA | 943 | | ILE | 2 | 70.624 | 45.977 | 13.162 | 1.00 29.29 | CPS2 |
| MOTA | 944 | C | ILE | 2 | 75.427 | 45.143 | 11.851 | 1.00 30.22 | CPS2 |
| ATOM | 945 | 0 | ILE | 2 | 75.785 | 46.098 | 11.157 | 1.00 29.17 | CPS2 |
| MOTA | 946 | N | TYR | 3 | 75.866 | 43.906 | 11.657 | 1.00 29.82 | CPS2 |
| MOTA | 947 | CA | TYR | 3 | 76.797 | 43.596 | 10.577 | 1.00 29.72 | CPS2 |
| ATOM | 948 | CB | TYR | 3 | 77.594 | 42.334 | 10.900 | 1.00 32.80 | CPS2 |
| ATOM | 949 | CG | TYR | 3 | 78.536 | 41.959 | 9.782 | 1.00 37.46 | CPS2 |
| MOTA | 950 | CD1 | | 3 | 79.553 | 42.827 | 9.394 | 1.00 39.59 | CPS2 |
| | 951 | CEI | TYR | 3 | 80.382 | 42.538 | 8.314 | 1.00 42.43 | CPS2 |
| ATOM | | | | | | | | 1.00 39.81 | CPS2 |
| MOTA | 952 | CD2 | | 3 | 78.370 | 40.775 | 9.064 | | |
| MOTA | 953 | CE2 | TYR | 3 | 79.196 | 40.470 | 7.974 | 1.00 42.42 | CPS2 |
| MOTA | 954 | CZ | TYR | 3 | 80.201 | 41.364 | 7.607 | 1.00 44.04 | CPS2 |
| MOTA | 955 | OH | TYR | 3 | 81.024 | 41.099 | 6.531 | 1.00 46.34 | CPS2 |
| ATOM | 956 | C | TYR | 3 | 76.032 | 43.379 | 9.275 | 1.00 28.30 | CPS2 |
| MOTA | 957 | 0 | TYR | 3 | 76.420 | 43.872 | 8.211 | 1.00 28.24 | CPS2 |
| ATOM | 958 | N | GLY | 4 | 74.944 | 42.619 | 9.363 | 1.00 25.87 | CPS2 |
| ATOM | 95 9 | CA | GLY | 4 | 74.141 | 42.355 | 8.182 | 1.00 22.75 | CPS2 |
| | | | | | | | | 1.00 21.62 | CPS2 |
| MOTA | 960 | C | GLY | 4 | 72.849 | 41.652 | 8.547 | 1.00 21.62 | CPS2 |
| ATOM | 961 | 0 | GLY | 4 | 72.724 | 41.085 | 9.639 | | |
| ATOM | 962 | N | ILE | 5 | 71.877 | 41.703 | 7.640 | 1.00 20.89 | CPS2 |
| MOTA | 963 | CA | ILE | 5 | 70.593 | 41.042 | 7.859 | 1.00 19.45 | CPS2 |
| ATOM | 964 | CB | ILE | 5 | 69.453 | 42.057 | 8.118 | 1.00 18.65 | CPS2 |
| ATOM | 965 | CG2 | ILE | 5 | 69.846 | 43.011 | 9.259 | 1.00 19.69 | CPS2 |
| MOTA | 966 | | ILE | 5 | 69.129 | 42.843 | 6.842 | 1.00 19.64 | CPS2 |
| ATOM | 967 | | ILE | 5 | 67.947 | 43.809 | 7.020 | 1.00 20.64 | CPS2 |
| | 968 | C | ILE | 5 | 70.272 | 40.216 | 6.618 | 1.00 18.82 | CPS2 |
| ATOM | 200 | _ | TUE | Э | 10.412 | 40.410 | 0.010 | 2.00 10.02 | |

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| MOTA | 969 | 0 | ILE | 5 | 70.778 | 40.498 | 5.524 | 1.00 18.88 | CPS2 |
|--------------|--------------|----------|------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 970 | N | GLY | 6 | 69.456 | 39.184 | 6.794 | 1.00 19.17 | CPS2 |
| MOTA | 971 | CA | GLY | 6 | 69.108 | 38.325 | 5.679 | 1.00 19.31 | CPS2 |
| MOTA | 972 | C | GLY | 6 | 67.687 | 37.815 | 5.794 | 1.00 19.36 | CPS2 |
| ATOM | 973 | 0 | GLY | 6 | 67.176 | 37.614 | 6.887 | 1.00 18.63 | CPS2 |
| MOTA | 974 | N | LEU | 7 | 67.053 | 37.606 | 4.649 | 1.00 19.78 | CPS2 |
| ATOM | 975 | CA | LEU | 7 | 65.680 | 37.141 | 4.617 | 1.00 19.08 | CPS2 |
| ATOM | 976 | CB | LEU | 7 | 64.733 | 38.328 | 4.366 | 1.00 19.19 | CPS2 |
| MOTA | 977 | CG | LEU | 7 | 63.238 | 38.018 | 4.161 | 1.00 18.29 | CPS2 |
| ATOM | 978 | | LEU | 7 | 62.658 | 37.539 | 5.491 | 1.00 18.90 | CPS2 |
| ATOM | 979 | | LEU | 7 | 62.472 | 39.269 | 3.651 | 1.00 17.44 | CPS2 |
| ATOM | 980 | C | LEU | 7 | 65.552 | 36.139 36.338 | 3.487 | 1.00 18.38 1.00 19.54 | CPS2 |
| MOTA | 981 | 0 | LEU ASP | 7 | 66.113 | | 2.417 | | CPS2 |
| ATOM ATOM | 982 983 | N CA | ASP | 8 8 | 64.845 64.651 | 35.042 34.091 | 3.724 2.647 | 1.00 18.51 1.00 20.25 | CPS2 CPS2 |
| ATOM | 984 | CB | ASP | 8 | 65.727 | 32.998 | 2.657 | 1.00 20.23 | CPS2 |
| ATOM | 985 | CG | ASP | 8 | 65.487 | 31.943 | 1.580 | 1.00 25.13 | CPS2 |
| ATOM | 986 | | ASP | 8 | 64.777 | 30.949 | 1.851 | 1.00 25.80 | CPS2 |
| ATOM | 987 | | ASP | 8 | 65.989 | 32.124 | 0.454 | 1.00 28.14 | CPS2 |
| MOTA | 988 | C | ASP | 8 | 63.297 | 33.433 | 2.740 | 1.00 20.84 | CPS2 |
| MOTA | 989 | Ō | ASP | 8 | 62.826 | 33.137 | 3.834 | 1.00 19.86 | CPS2 |
| ATOM | 990 | N | ILE | 9 | 62.669 | 33.223 | 1.584 | 1.00 19.61 | CPS2 |
| ATOM | 991 | CA | ILE | 9 | 61.391 | 32.520 | 1.533 | 1.00 20.19 | CPS2 |
| MOTA | 992 | CB | ILE | 9 | 60.222 | 33.393 | 1.015 | 1.00 21.26 | CPS2 |
| ATOM | 993 | CG2 | ILE | 9 | 58.950 | 32.526 | 0.904 | 1.00 20.13 | CPS2 |
| ATOM | 994 | CG1 | ILE | 9 | 59.959 | 34.555 | 1.973 | 1.00 21.42 | CPS2 |
| MOTA | 995 | CD1 | ILE | 9 | 58.878 | 35.500 | 1.490 | 1.00 21.37 | CPS2 |
| MOTA | 996 | C | ILE | 9 | 61.641 | 31.415 | 0.519 | 1.00 20.37 | CPS2 |
| MOTA | 997 | 0 | ILE | 9 | 62.132 | 31.685 | -0.572 | 1.00 20.53 | CPS2 |
| ATOM | 998 | N | THR | 10 | 61.313 | 30.182 | 0.892 | 1.00 20.80 | CPS2 |
| MOTA | 999 | CA | THR | 10 | 61.519 | 29.032 | 0.022 | 1.00 22.14 | CPS2 |
| MOTA | 1000 | CB | THR | 10 | 62.584 | 28.076 | 0.630 | 1.00 23.02 | CPS2 |
| ATOM | 1001 | OG1 | | 10 | 63.837 | 28.770 | 0.746 | 1.00 25.04 | CPS2 |
| MOTA | 1002 | CG2 | | 10 | 62.785 | 26.859 | -0.253 | 1.00 25.37 | CPS2 |
| ATOM | 1003 | C | THR | 10 | 60.211 | 28.275 | -0.184 | 1.00 21.99 | CPS2 |
| ATOM | 1004 | 0 | THR | 10 | 59.471 | 28.038 | 0.761 | 1.00 21.01 1.00 23.31 | CPS2 CPS2 |
| MOTA | 1005 | N | GLU | 11 | 59.938 | 27.912 | -1.435 | 1.00 23.31 | CPS2 |
| ATOM | 1006 | CA | GLU | 11 | 58.723 | 27.177 27.355 | -1.794 -3.296 | 1.00 24.42 | CPS2 |
| ATOM | 1007 | CB CG | GLU | 11 11 | 58.438 57.052 | 26.900 | -3.721 | 1.00 28.32 | CPS2 |
| ATOM | 1008 1009 | CD | GLU | 11 | 56.897 | 26.756 | -5.231 | 1.00 32.57 | CPS2 |
| ATOM ATOM | 1010 | | GLU | 11 | 57.820 | 27.134 | -5.991 | 1.00 32.18 | CPS2 |
| ATOM | 1011 | _ | GLU | 11 | 55.833 | 26.256 | -5.654 | 1.00 33.69 | CPS2 |
| ATOM | 1012 | C | GLU | 11 | 58.941 | 25.692 | -1.480 | 1.00 23.56 | CPS2 |
| MOTA | 1013 | ō | GLU | 11 | 59.853 | 25.070 | -2.026 | 1.00 22.90 | CPS2 |
| ATOM | 1014 | N | LEU | 12 | 58.110 | 25.124 | -0.612 | 1.00 23.91 | CPS2 |
| ATOM | 1015 | CA | LEU | 12 | 58.260 | 23.715 | -0.249 | 1.00 26.06 | CPS2 |
| ATOM | 1016 | CB | LEU | 12 | 57.147 | 23.269 | 0.705 | 1.00 28.23 | CPS2 |
| ATOM | 1017 | ÇG | LEU | 12 | 57.554 | 23.114 | 2.176 | 1.00 31.10 | CPS2 |
| ATOM | 1018 | | LEU | 12 | 58.046 | 24.448 | 2.710 | 1.00 30.63 | CPS2 |
| ATOM | 1019 | - | LEU | 12 | 56.360 | 22.605 | 3.005 | 1.00 32.22 | CPS2 |
| ATOM | 1020 | C | LEU | 12 | 58.271 | 22.795 | -1.461 | 1.00 27.56 | CPS2 |
| ATOM | 1021 | ō | LEU | 12 | 59.054 | 21.846 | -1.519 | 1.00 27.33 | CPS2 |
| ATOM | 1022 | N | ALA | 13 | 57.401 | 23.077 | -2.427 | 1.00 27.64 | CPS2 |
| ATOM | 1023 | CA | ALA | 13 | 57.321 | 22.255 | -3.628 | 1.00 28.06 | CPS2 |
| ATOM | 1024 | CB | ALA | 13 | 56.163 | 22.714 | -4.506 | 1.00 28.61 | CPS2 |
| ATOM | 1025 | С | ALA | 13 | 58.622 | 22.279 | -4.413 | 1.00 29.21 | CPS2 |
| | | | | | | | | | |

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| MOTA | 1026 | 0 | ALA | 13 | 58.982 | 21.281 | -5.048 | 1.00 28.52 | CPS2 |
|------|------|-----|-----|----|--------|---------|---------|------------|------|
| ATOM | 1027 | N | ARG | 14 | 59.335 | 23.404 | -4.375 | 1.00 29.11 | CPS2 |
| ATOM | 1028 | CA | ARG | 14 | 60.599 | 23.495 | -5.098 | 1.00 30.50 | CPS2 |
| MOTA | 1029 | CB | ARG | 14 | 61.065 | 24.951 | -5.221 | 1.00 32.06 | CPS2 |
| ATOM | 1030 | CG | ARG | 14 | 62.248 | 25.118 | -6.171 | 1.00 34.92 | CPS2 |
| ATOM | 1031 | CD | ARG | 14 | 62.528 | 26.576 | -6.477 | 1.00 34.32 | CPS2 |
| MOTA | 1032 | NE | ARG | 14 | 63.217 | 27.245 | -5.381 | 1.00 38.47 | CPS2 |
| ATOM | 1032 | CZ | ARG | 14 | 64.522 | | | | |
| | | | | | | 27.137 | -5.142 | 1.00 39.99 | CPS2 |
| ATOM | 1034 | NH1 | | 14 | 65.284 | 26.385 | -5.926 | 1.00 39.47 | CPS2 |
| ATOM | 1035 | NH2 | | 14 | 65.066 | 27.787 | -4.119 | 1.00 39.80 | CPS2 |
| MOTA | 1036 | C | ARG | 14 | 61.670 | 22.655 | -4.411 | 1.00 30.84 | CPS2 |
| ATOM | 1037 | 0 | ARG | 14 | 62.488 | 22.021 | -5.077 | 1.00 31.28 | CPS2 |
| ATOM | 1038 | N | ILE | 15 | 61.672 | 22.650 | -3.078 | 1.00 31.04 | CPS2 |
| MOTA | 1039 | CA | ILE | 15 | 62.637 | 21.845 | -2.332 | 1.00 31.02 | CPS2 |
| MOTA | 1040 | CB | ILE | 15 | 62.480 | 22.037 | -0.803 | 1.00 30.76 | CPS2 |
| MOTA | 1041 | CG2 | ILE | 15 | 63.314 | 21.002 | -0.056 | 1.00 29.83 | CPS2 |
| MOTA | 1042 | CGl | ILE | 15 | 62.940 | 23.441 | -0.407 | 1.00 29.97 | CPS2 |
| MOTA | 1043 | CD1 | ILE | 15 | 64.431 | 23.685 | -0.657 | 1.00 30.60 | CPS2 |
| ATOM | 1044 | C | ILE | 15 | 62.397 | 20.369 | -2.673 | 1.00 33.28 | CPS2 |
| ATOM | 1045 | 0 | ILE | 15 | 63.338 | 19.604 | -2.900 | 1.00 33.51 | CPS2 |
| ATOM | 1046 | N | ALA | 16 | 61.133 | 19.974 | -2.712 | 1.00 34.78 | CPS2 |
| ATOM | 1047 | CA | ALA | 16 | 60.789 | 18.597 | -3.039 | 1.00 37.29 | CPS2 |
| ATOM | 1048 | CB | ALA | 16 | 59.285 | 18.395 | -2.921 | 1.00 36.48 | CPS2 |
| ATOM | 1049 | C | ALA | 16 | 61.264 | 18.286 | -4.459 | 1.00 39.28 | CPS2 |
| ATOM | 1050 | 0 | ALA | 16 | 61.839 | 17.230 | -4.716 | 1.00 40.75 | CPS2 |
| ATOM | 1051 | N | SER | 17 | 61.034 | 19.219 | -5.375 | 1.00 40.88 | CPS2 |
| ATOM | 1052 | CA | SER | 17 | 61.439 | 19.046 | -6.763 | 1.00 43.46 | CPS2 |
| MOTA | 1053 | CB | SER | 17 | 61.012 | 20.261 | -7.588 | 1.00 44.13 | CPS2 |
| MOTA | 1054 | OG | SER | 17 | 61.450 | 20.150 | -8.930 | 1.00 46.75 | CPS2 |
| MOTA | 1055 | C | SER | 17 | 62.949 | 18.857 | -6.866 | 1.00 44.93 | CPS2 |
| ATOM | 1056 | Ö | SER | 17 | 63.432 | 18.058 | -7.672 | 1.00 44.94 | CPS2 |
| ATOM | 1057 | N | MET | 18 | 63.694 | 19.597 | -6.052 | 1.00 45.72 | CPS2 |
| ATOM | 1058 | CA | MET | 18 | 65.148 | 19.499 | -6.060 | 1.00 47.01 | CPS2 |
| ATOM | 1059 | CB | MET | 18 | 65.780 | 20.713 | -5.374 | 1.00 47.40 | CPS2 |
| ATOM | 1060 | CG | MET | 18 | 65.783 | 21.978 | -6.201 | 1.00 47.40 | CPS2 |
| | 1061 | SD | MET | 18 | 66.874 | 23.231 | -5.488 | 1.00 48.01 | CPS2 |
| ATOM | | | | | | | | | CPS2 |
| ATOM | 1062 | CE | MET | 18 | 65.856 | 23.843 | -4.148 | 1.00 49.70 | |
| MOTA | 1063 | C | MET | 18 | 65.637 | 18.233 | ~5.369 | 1.00 47.60 | CPS2 |
| MOTA | 1064 | 0 | MET | 18 | 66.589 | 17.605 | -5.822 | 1.00 48.05 | CPS2 |
| MOTA | 1065 | N | ALA | 19 | 64.982 | 17.863 | -4.275 | 1.00 48.91 | CPS2 |
| MOTA | 1066 | CA | ALA | 19 | 65.365 | 16.682 | -3.512 | 1.00 50.86 | CPS2 |
| MOTA | 1067 | CB | ALA | 19 | 64.590 | 16.637 | -2.209 | 1.00 50.39 | CPS2 |
| ATOM | 1068 | C | ALA | 19 | 65.135 | 15.396 | -4.296 | 1.00 53.04 | CPS2 |
| ATOM | 1069 | 0 | ALA | 19 | 65.897 | 14.433 | -4.171 | 1.00 52.81 | CPS2 |
| ATOM | 1070 | N | GLY | 20 | 64.084 | 15.384 | -5.108 | 1.00 54.91 | CPS2 |
| MOTA | 1071 | CA | GLY | 20 | 63.773 | 14.201 | -5.888 | 1.00 56.86 | CPS2 |
| ATOM | 1072 | C | GLY | 20 | 64.693 | 13.980 | -7.072 | 1.00 58.24 | CPS2 |
| MOTA | 1073 | 0 | GLY | 20 | 65.285 | 12.909 | -7.217 | 1.00 58.99 | CPS2 |
| ATOM | 1074 | N | ARG | 21 | 64.827 | 14.996 | -7.916 | 1.00 59.32 | CPS2 |
| MOTA | 1075 | CA | ARG | 21 | 65.652 | 14.882 | -9.107 | 1.00 60.71 | CPS2 |
| MOTA | 1076 | CB | ARG | 21 | 65.279 | 15.975 | -10.112 | 1.00 61.88 | CPS2 |
| MOTA | 1077 | CG | ARG | 21 | 65.739 | 17.362 | -9.716 | 1.00 63.83 | CPS2 |
| MOTA | 1078 | CD | ARG | 21 | 65.818 | 18.274 | -10.930 | 1.00 65.39 | CPS2 |
| ATOM | 1079 | NE | ARG | 21 | 66.617 | 19.471 | -10.669 | 1.00 67.17 | CPS2 |
| ATOM | 1080 | CZ | ARG | 21 | 66.250 | 20.467 | -9.867 | 1.00 67.54 | CPS2 |
| ATOM | 1081 | | ARG | 21 | 65.082 | 20.423 | -9.237 | 1.00 68.19 | CPS2 |
| ATOM | 1082 | | ARG | 21 | 67.057 | 21.507 | | 1.00 67.30 | CPS2 |
| 01.1 | | | | | 3,.00, | ,,,,,,, | 2.020 | | |

| MOTA | 1083 | C | ARG | 21 | 67.153 | 14.932 | -8.857 | 1.00 61.11 | CPS2 |
|----------|------|-----|-----|------------|----------------|--------|--------|------------|------|
| MOTA | 1084 | 0 | ARG | 21 | 67.942 | 14.571 | -9.735 | 1.00 61.28 | CPS2 |
| MOTA | 1085 | N | GLN | 22 | 67.564 | 15.375 | -7.674 | 1.00 61.25 | CPS2 |
| ATOM | 1086 | CA | GLN | 22 | 68.994 | 15.461 | -7.402 | 1.00 60.88 | CPS2 |
| MOTA | 1087 | CB | GLN | 22 | 69.340 | 16.826 | -6.795 | 1.00 61.70 | CPS2 |
| MOTA | 1088 | CG | GLN | 22 | 69.033 | 17.998 | -7.722 | 1.00 62.47 | CPS2 |
| ATOM | 1089 | CD | GLN | 22 | 69.522 | 19.331 | -7.180 | 1.00 63.25 | CPS2 |
| ATOM | 1090 | OE1 | GLN | 22 | 69.279 | 20.381 | -7.779 | 1.00 63.34 | CPS2 |
| MOTA | 1091 | NE2 | GLN | 22 | 70.218 | 19.297 | -6.047 | 1.00 63.02 | CPS2 |
| MOTA | 1092 | С | GLN | 22 | 69.563 | 14.351 | -6.530 | 1.00 60.08 | CPS2 |
| ATOM | 1093 | 0 | GLN | 22 | 68.836 | 13.608 | -5.867 | 1.00 60.33 | CPS2 |
| MOTA | 1094 | N | LYS | 23 | 70.886 | 14.253 | -6.569 | 1.00 59.12 | CPS2 |
| ATOM | 1095 | CA | LYS | 23 | 71.665 | 13.273 | -5.823 | 1.00 57.97 | CPS2 |
| ATOM | 1096 | CB | LYS | 23 | 73.13 7 | 13.684 | -5.890 | 1.00 59.44 | CPS2 |
| MOTA | 1097 | CG | LYS | 23 | 73.362 | 15.214 | -5.851 | 1.00 60.21 | CPS2 |
| MOTA | 1098 | CD | LYS | 23 | 73.057 | 15.850 | -4.501 | 1.00 59.91 | CPS2 |
| ATOM | 1099 | CE | LYS | 23 | 73.391 | 17.340 | -4.455 | 1.00 60.70 | CPS2 |
| ATOM | 1100 | NZ | LYS | 23 | 72.466 | 18.181 | -5.268 | 1.00 59.44 | CPS2 |
| MOTA | 1101 | C | LYS | 23 | 71.253 | 13,118 | -4.360 | 1.00 56.31 | CPS2 |
| ATOM | 1102 | Ō | LYS | 23 | 70.226 | 12.517 | -4.027 | 1.00 57.13 | CPS2 |
| ATOM | 1103 | N | ARG | 24 | 72.112 | 13.635 | -3.496 | 1.00 53.19 | CPS2 |
| MOTA | 1104 | CA | ARG | 24 | 71.909 | 13.629 | -2.062 | 1.00 50.41 | CPS2 |
| ATOM | 1105 | CB | ARG | 24 | 73.117 | 12.987 | -1.365 | 1.00 51.60 | CPS2 |
| ATOM | 1106 | CG | ARG | 24 | 74.311 | 12.739 | -2.286 | 1.00 51.97 | CPS2 |
| ATOM | 1107 | CD | ARG | 24 | 75.442 | 12.014 | -1.565 | 1.00 52.64 | CPS2 |
| ATOM | 1108 | NE | ARG | 24 | 75.105 | 10.634 | -1.218 | 1.00 51.83 | CPS2 |
| ATOM | 1109 | CZ | ARG | 24 | 75.534 | 9.570 | -1.892 | 1.00 51.87 | CPS2 |
| ATOM | 1110 | | ARG | 24 | 76.318 | 9.728 | -2.950 | 1.00 51.30 | CPS2 |
| ATOM | 1111 | | ARG | 24 | 75.187 | 8.347 | -1.505 | 1.00 51.09 | CPS2 |
| ATOM | 1112 | C | ARG | 24 | 71.787 | 15.110 | -1.717 | 1.00 47.01 | CPS2 |
| ATOM | 1113 | ō | ARG | 24 | 72.640 | 15.690 | -1.043 | 1.00 46.57 | CPS2 |
| MOTA | 1114 | N | PHE | 25 | 70.725 | 15.721 | -2.238 | 1.00 42.31 | CPS2 |
| ATOM | 1115 | CA | PHE | 25 | 70.450 | 17.134 | -2.019 | 1.00 38.57 | CPS2 |
| ATOM | 1116 | CB | PHE | 25 | 69.115 | 17.508 | -2.679 | 1.00 37.72 | CPS2 |
| ATOM | 1117 | CG | PHE | 25 | 68.680 | 18.926 | -2.416 | 1.00 36.40 | CPS2 |
| ATOM | 1118 | CD1 | | 25 | 67.682 | 19.202 | -1.485 | 1.00 36.71 | CPS2 |
| ATOM | 1119 | CD2 | PHE | 25 | 69.285 | 19.986 | -3.080 | 1.00 37.10 | CPS2 |
| ATOM | 1120 | | PHE | 25 | 67.297 | 20.518 | -1,220 | 1.00 36.02 | CPS2 |
| ATOM | 1121 | | PHE | 25 | 68.910 | 21.305 | -2.824 | 1.00 35.88 | CPS2 |
| ATOM | 1122 | CZ | PHE | 25 | 67.914 | 21.572 | -1.891 | 1.00 36.06 | CPS2 |
| ATOM | 1123 | C | PHE | 25 | 70.415 | 17.465 | -0.528 | 1.00 36.15 | CPS2 |
| ATOM | 1124 | Ō | PHE | 25 | 71.053 | 18.423 | -0.079 | 1.00 35.69 | CPS2 |
| ATOM | 1125 | N | ALA | 26 | 69.671 | 16.664 | 0.228 | 1.00 33.10 | CPS2 |
| ATOM | 1126 | CA | ALA | 26 | 69.548 | 16.865 | 1.667 | 1.00 32.04 | CPS2 |
| MOTA | 1127 | CB | ALA | 26 | 68.663 | 15.780 | 2.270 | 1.00 30.86 | CPS2 |
| ATOM | 1128 | c | ALA | 26 | 70.931 | 16.835 | 2.312 | 1.00 31.57 | CPS2 |
| ATOM | 1129 | ō | ALA | 26 | 71.249 | 17.655 | 3.180 | 1.00 28.07 | CPS2 |
| MOTA | 1130 | N | GLU | 27 | 71.747 | 15.881 | 1.868 | 1.00 29.98 | CPS2 |
| ATOM | 1131 | CA | GLU | 27 | 73.102 | 15.717 | 2.382 | 1.00 30.25 | CPS2 |
| ATOM | 1132 | CB | GLU | 27 | 73.745 | 14.457 | 1.794 | 1.00 31.17 | CPS2 |
| ATOM | 1133 | CG | GLU | 27 | 73.219 | 13.134 | 2.356 | 1.00 35.24 | CPS2 |
| ATOM | 1134 | CD | GLU | 27 | 71.772 | 12.823 | 1.978 | 1.00 37.65 | CPS2 |
| ATOM | 1135 | | GLU | 27 | 71.772 | 13.296 | 0.918 | 1.00 38.95 | CPS2 |
| ATOM | 1136 | | GLU | 27 | 71.113 | 12.076 | 2.742 | 1.00 40.73 | CPS2 |
| ATOM | 1137 | C | GLU | 27 | 73.974 | 16.925 | 2.063 | 1.00 28.88 | CPS2 |
| ATOM | 1137 | 0 | GLU | 27 | 74.879 | 17.254 | 2.823 | 1.00 28.66 | CPS2 |
| ATOM | 1138 | и | ARG | 28 | 73.705 | 17.578 | 0.935 | 1.00 27.77 | CPS2 |
| 227 02.7 | | ~• | | - • | | 2 | | | |

| MOTA | 1140 | CA | ARG | 28 | 74.470 | 18.754 | 0.532 | 1.00 29.47 | CPS2 |
|--------------|--------------|-----------|------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 1141 | CB | ARG | 28 | 74.201 | 19.076 | -0.948 | 1.00 30.98 | CPS2 |
| ATOM | 1142 | CG | ARG | 28 | 74.785 | 20.407 | -1.424 | 1.00 35.00 | CPS2 |
| ATOM | 1143 | CD | ARG | 28 | 74.806 | 20.528 | -2.953 | 1.00 38.43 | CPS2 |
| ATOM | 1144 | NE | ARG | 28 | 73.480 | 20.654 | -3.557 | 1.00 40.71 | CPS2 |
| ATOM | 1145 | CZ | ARG | 28 | 72.809 | 21.797 | -3.683 | 1.00 42.27 | CPS2 |
| MOTA | 1146 | NH1 | ARG | 28 | 73.327 | 22.940 | -3.248 | 1.00 42.45 | CPS2 |
| ATOM | 1147 | NH2 | ARG | 28 | 71.613 | 21.798 | -4.259 | 1.00 44.17 | CPS2 |
| ATOM | 1148 | С | ARG | 28 | 74.137 | 19.987 | 1.387 | 1.00 28.50 | CPS2 |
| MOTA | 1149 | 0 | ARG | 28 | 75.003 | 20.811 | 1.669 | 1.00 29.58 | CPS2 |
| ATOM | 1150 | N | ILE | 29 | 72.879 | 20.105 | 1.788 | 1.00 26.47 | CPS2 |
| ATOM | 1151 | CA | ILE | 29 | 72.426 | 21.256 | 2.570 | 1.00 26.32 | CPS2 |
| ATOM | 1152 | CB | ILE | 29 | 70.908 | 21.475 | 2.389 | 1.00 25.79 | CPS2 |
| MOTA | 1153 | CG2 | ILE | 29 | 70.467 | 22.729 | 3.147 | 1.00 24.32 | CPS2 |
| ATOM | 1154 | CG1 | ILE | 29 | 70.559 | 21.566 | 0.902 | 1.00 23.95 | CPS2 |
| MOTA | 1155 | CD1 | ILE | 29 | 71.283 | 22.665 | 0.158 | 1.00 26.12 | CPS2 |
| MOTA | 1156 | C | ILE | 29 | 72.681 | 21.128 | 4.064 | 1.00 26.65 | CPS2 |
| MOTA | 1157 | 0 | ILE | 29 | 73.024 | 22.110 | 4.739 | 1.00 26.47 | CPS2 |
| ATOM | 1158 | N | LEU | 30 | 72.516 | 19.908 | 4.566 | 1.00 26.29 | CPS2 |
| ATOM | 1159 | CA | LEU | 30 | 72.638 | 19.616 | 5.981 | 1.00 26.30 | CPS2 |
| ATOM | 1160 | CB | LEU | 30 | 71.518 | 18.645 | 6.371 | 1.00 26.05 | CPS2 |
| ATOM | 1161 | CG | LEU | 30 | 70.095 | 19.059 | 5.957 | 1.00 26.30 | CPS2 |
| ATOM | 1162 | | LEU | 30 | 69.081 | 18.002 | 6.387 | 1.00 26.56 | CPS2 |
| ATOM | 1163 | CD2 | LEU | 30 | 69.762 | 20.400 | 6.602 | 1.00 24.24 | CPS2 |
| ATOM | 1164 | C | LEU | 30 | 73.972 | 19.075 | 6.497 | 1.00 27.26 | CPS2 |
| ATOM | 1165 | 0 | LEU | 30 | 74.731 | 18.419 | 5.771 | 1.00 28.28 | CPS2 |
| ATOM | 1166 | N | THR | 31 | 74.246 | 19.372 | 7.765 | 1.00 26.23 | CPS2 |
| MOTA | 1167 | CA | THR | 31 | 75.451 | 18.898 | 8.434 | 1.00 26.09 | CPS2 |
| MOTA | 1168 | CB | THR | 31 | 75.844 | 19.806 | 9.627 | 1.00 24.78 | CPS2 |
| MOTA | 1169 | OG1 | | 31 | 74.834 | 19.723 | 10.638 | 1.00 25.44 | CPS2 |
| MOTA | 1170 | CG2 | | 31 | 75.998 | 21.253 | 9.172 | 1.00 25.52 | CPS2 |
| MOTA | 1171 | C | THR | 31 | 75.106 | 17.516 | 8.978 | 1.00 26.34 | CPS2 |
| MOTA | 1172 | 0 | THR | 31 | 73.945 | 17.106 | 8.956 | 1.00 25.24 | CPS2 |
| ATOM | 1173 | N | ARG | 32 | 76.108 | 16.791 | 9.463 | 1.00 28.14 | CPS2 |
| ATOM | 1174 | CA | ARG | 32 | 75.872 | 15.456 | 10.005 | 1.00 30.16 | CPS2 |
| ATOM | 1175 | CB | ARG | 32 | 77.195 | 14.862 | 10.519 | 1.00 32.90 | CPS2 CPS2 |
| ATOM | 1176 | CG | ARG | 32 | 77.070 | 13.518 | 11.243 | 1.00 37.77 | CPS2 |
| MOTA | 1177 | CD | ARG | 32 | 78.452 | 13.018 12.082 | 11.667 | 1.00 42.29 1.00 46.64 | CPS2 |
| ATOM | 1178 | NE | ARG | 32 | 78.428 | 10.817 | 12.796 12.728 | 1.00 48.51 | CPS2 |
| MOTA MOTA | 1179 1180 | CZ NH1 | ARG ARG | 32 32 | 78.020 77.588 | 10.314 | 11.581 | 1.00 48.31 | CPS2 |
| MOTA | 1181 | | ARG | 32 | 78.058 | 10.045 | 13.809 | 1.00 49.25 | CPS2 |
| MOTA | 1182 | C | ARG | 32 | 74.812 | 15.450 | 11.116 | 1.00 29.69 | CPS2 |
| ATOM | 1183 | 0 | ARG | 32 | 73.946 | 14.577 | 11.149 | 1.00 29.33 | CPS2 |
| ATOM | 1184 | N | SER | 33 | 74.858 | 16.428 | 12.019 | 1.00 29.98 | CPS2 |
| ATOM | 1185 | CA | SER | 33 | 73.886 | 16.473 | 13.112 | 1.00 29.46 | CPS2 |
| ATOM | 1186 | CB | SER | 33 | 74.338 | 17.475 | 14.180 | 1.00 32.61 | CPS2 |
| ATOM | 1187 | OG | SER | 33 | 74.402 | 18.784 | 13.645 | 1.00 37.61 | CPS2 |
| ATOM | 1188 | C | SER | 33 | 72.464 | 16.813 | 12.652 | 1.00 28.59 | CPS2 |
| ATOM | 1189 | o | SER | 33 | 71.488 | 16.317 | 13.211 | 1.00 27.50 | CPS2 |
| MOTA | 1190 | N | GLU | 34 | 72.345 | 17.682 | 11.654 | 1.00 27.39 | CPS2 |
| ATOM | 1191 | CA | GLU | 34 | 71.036 | 18.051 | 11.131 | 1.00 27.27 | CPS2 |
| MOTA | 1192 | CB | GLU | 34 | 71.178 | 19.215 | 10.140 | 1.00 26.09 | CPS2 |
| ATOM | 1193 | CG | GLU | 34 | 71.493 | 20.554 | 10.824 | 1.00 27.08 | CPS2 |
| ATOM | 1194 | CD | GLU | 34 | 71.939 | 21.642 | 9.860 | 1.00 27.39 | CPS2 |
| ATOM | 1195 | | . GLU | 34 | 71.813 | 22.838 | 10.220 | 1.00 26.38 | CPS2 |
| ATOM | 1196 | | GLU | 34 | 72.427 | 21.310 | 8.755 | 1.00 25.66 | CPS2 |
| | | | | | | | | | |

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| ATOM | 1197 | C | GLU | 34 | 70.443 | 16.828 | 10.437 | 1.00 27.36 | CPS2 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| ATOM | 1198 | 0 | GLU | 34 | 69.239 | 16.562 | 10.532 | 1.00 26.33 | CPS2 |
| ATOM | 1199 | N | LEU | 35 | 71.302 | 16.077 | 9.750 | 1.00 28.28 | CPS2 |
| ATOM | 1200 | CA | LEU | 35 | 70.862 | 14.877 | 9.045 | 1.00 29.11 | |
| ATOM | 1201 | CB | LEU | 35 | | | | | CPS2 |
| | | | | | 72.021 | 14.251 | 8.270 | 1.00 28.46 | CPS2 |
| ATOM | 1202 | CG | LEU | 35 | 72.336 | 14.922 | 6.940 | 1.00 27.65 | CPS2 |
| MOTA | 1203 | | LEU | 35 | 73.659 | 14.380 | 6.379 | 1.00 29.47 | CPS2 |
| MOTA | 1204 | CD2 | LEU | 35 | 71.182 | 14.664 | 5.965 | 1.00 28.02 | CPS2 |
| MOTA | 1205 | C | LEU | 35 | 70.281 | 13.851 | 9.998 | 1.00 30.80 | CPS2 |
| MOTA | 1206 | 0 | LEU | 35 | 69.303 | 13.191 | 9.668 | 1.00 31.95 | CPS2 |
| ATOM | 1207 | N | ASP | 36 | 70.883 | 13.709 | 11.175 | 1.00 32.92 | CPS2 |
| ATOM | 1208 | CA | ASP | 36 | 70.380 | 12.756 | 12.161 | 1.00 35.31 | CPS2 |
| ATOM | 1209 | CB | ASP | 36 | 71.247 | 12.759 | 13.416 | 1.00 38.59 | CPS2 |
| ATOM | 1210 | CG | ASP | 36 | 72.527 | 11.974 | 13.236 | 1.00 43.41 | CPS2 |
| ATOM | 1211 | | ASP | 36 | 72.449 | 10.838 | 12.713 | 1.00 47.13 | CPS2 |
| | | | | 36 | | | | | |
| ATOM | 1212 | | ASP | | 73.606 | 12.480 | 13.618 | 1.00 45.83 | CPS2 |
| ATOM | 1213 | C | ASP | 36 | 68.948 | 13.107 | 12.531 | 1.00 35.32 | CPS2 |
| MOTA | 1214 | 0 | ASP | 36 | 68.108 | 12.228 | 12.733 | 1.00 35.28 | CPS2 |
| MOTA | 1215 | N | GLN | 37 | 68.675 | 14.404 | 12.621 | 1.00 34.28 | CPS2 |
| ATOM | 1216 | CA | GLN | 37 | 67.338 | 14.881 | 12.945 | 1.00 32.79 | CPS2 |
| MOTA | 1217 | CB | GLN | 37 | 67.401 | 16.378 | 13.297 | 1.00 33.92 | CPS2 |
| ATOM | 1218 | CG | GLN | 37 | 68.022 | 16.651 | 14.662 | 1.00 35.15 | CPS2 |
| ATOM | 1219 | CD | GLN | 37 | 68.443 | 18.110 | 14.876 | 1.00 36.52 | CPS2 |
| ATOM | 1220 | OE1 | GLN | 37 | 68.733 | 18.517 | 16.001 | 1.00 37.53 | CPS2 |
| ATOM | 1221 | | GLN | 37 | 68.495 | 18.887 | 13.799 | 1.00 34.94 | CPS2 |
| ATOM | 1222 | C | GLN | 37 | 66.431 | 14.645 | 11.733 | 1.00 32.14 | CPS2 |
| ATOM | 1223 | 0 | GLN | 37 | 65.284 | 14.214 | 11.863 | 1.00 31.52 | CPS2 |
| ATOM | 1224 | И | TYR | 38 | 66.971 | 14.914 | 10.552 | 1.00 30.64 | CPS2 |
| | | | | | | | | | |
| ATOM | 1225 | CA | TYR | 38 | 66.239 | 14.753 | 9.307 | 1.00 30.51 | CPS2 |
| MOTA | 1226 | CB | TYR | 38 | 67.112 | 15.245 | 8.148 | 1.00 29.87 | CPS2 |
| MOTA | 1227 | CG | TYR | 38 | 66.544 | 15.040 | 6.762 | 1.00 30.29 | CPS2 |
| MOTA | 1228 | | TYR | 38 | 66.975 | 13.983 | 5.957 | 1.00 31.01 | CPS2 |
| MOTA | 1229 | | TYR | 38 | 66.500 | 13.829 | 4.653 | 1.00 31.49 | CPS2 |
| MOTA | 1230 | CD2 | TYR | 38 | 65.614 | 15.935 | 6.231 | 1.00 30.83 | CPS2 |
| ATOM | 1231 | CE2 | TYR | 38 | 65.135 | 15.792 | 4.938 | 1.00 31.82 | CPS2 |
| ATOM | 1232 | CZ | TYR | 38 | 65.582 | 14.742 | 4.153 | 1.00 32.74 | CPS2 |
| MOTA | 1233 | OH | TYR | 38 | 65.116 | 14.623 | 2.868 | 1.00 33.33 | CPS2 |
| MOTA | 1234 | C | TYR | 38 | 65.802 | 13.308 | 9.064 | 1.00 31.79 | CPS2 |
| ATOM | 1235 | 0 | TYR | 38 | 64.631 | 13.048 | 8.773 | 1.00 30.55 | CPS2 |
| ATOM | 1236 | N | TYR | 39 | 66.739 | 12.372 | 9.190 | 1.00 31.62 | CPS2 |
| ATOM | 1237 | CA | TYR | 39 | 66.423 | 10.965 | 8.946 | 1.00 33.46 | CPS2 |
| ATOM | 1238 | CB | TYR | 39 | 67.675 | 10.096 | 9.077 | 1.00 31.46 | CPS2 |
| | 1239 | CG | TYR | 39 | 68.760 | 10.350 | | 1.00 30.99 | CPS2 |
| MOTA | | | | _ | | | | | |
| MOTA | 1240 | | TYR | 39 | 68.449 | 10.548 | 6.702 | 1.00 31.00 | CPS2 |
| MOTA | 1241 | | TYR | 39 | 69.458 | 10.707 | 5.744 | 1.00 31.73 | CPS2 |
| ATOM | 1242 | | TYR | 39 | 70.108 | 10.321 | 8.413 | 1.00 32.22 | CPS2 |
| ATOM | 1243 | CE2 | TYR | 39 | 71.125 | 10.474 | 7.468 | 1.00 32.57 | CPS2 |
| ATOM | 1244 | CZ | TYR | 39 | 70.795 | 10.665 | 6.137 | 1.00 32.96 | CPS2 |
| ATOM | 1245 | OH | TYR | 39 | 71.813 | 10.784 | 5.211 | 1.00 33.59 | CPS2 |
| ATOM | 1246 | C | TYR | 39 | 65.331 | 10.411 | 9.862 | 1.00 34.30 | CPS2 |
| ATOM | 1247 | 0 | TYR | 39 | 64.653 | 9.451 | 9.506 | 1.00 35.26 | CPS2 |
| ATOM | 1248 | N | GLU | 40 | 65.155 | 11.015 | 11.030 | 1.00 36.00 | CPS2 |
| ATOM | 1249 | CA | GLU | 40 | 64.144 | 10.555 | 11.980 | 1.00 38.47 | CPS2 |
| MOTA | 1250 | CB | GLU | 40 | 64.468 | 11.069 | 13.387 | 1.00 41.11 | CPS2 |
| | | | | | | | 14.052 | 1.00 46.35 | CPS2 |
| ATOM | 1251 | CG | GLU | 40 | 65.650 | 10.394 | | | CPS2 |
| MOTA | 1252 | CD | GLU | 40 | 65.427 | 8.903 | 14.247 | | CPS2 |
| ATOM | 1253 | OEI | GLU | 40 | 64.505 | 8.527 | 15.006 | 1.00 50.90 | CF32 |
| | | | | | | | | | |

| MOTA | 1254 | OE2 | GLU | 40 | 66.174 | 8.108 | 13.632 | 1.00 51.72 | CPS2 |
|------|------|---------|-----|----------|------------------|--------|----------------|--------------------------|--------------|
| ATOM | 1255 | C | GLU | 40 | 62.720 | 10.980 | 11.631 | 1.00 38.59 | CPS2 |
| MOTA | 1256 | 0 | GLU | 40 | 61.761 | 10.472 | 12.210 | 1.00 38.70 | CPS2 |
| MOTA | 1257 | N | LEU | 41 | 62.579 | 11.905 | 10.688 | 1.00 37.33 | CPS2 |
| ATOM | 1258 | CA | LEU | 41 | 61.262 | 12.409 | 10.318 | 1.00 37.21 | CPS2 |
| ATOM | 1259 | CB | LEU | 41 | 61.371 | 13.881 | 9.908 | 1.00 36.12 | CPS2 |
| MOTA | 1260 | CG | LEU | 41 | 61.978 | 14.843 | 10.928 | 1.00 35.44 | CPS2 |
| ATOM | 1261 | CD1 | LEU | 41 | 62.095 | 16.224 | 10.296 | 1.00 35.33 | CPS2 |
| MOTA | 1262 | CD2 | LEU | 41 | 61.110 | 14.897 | 12.175 | 1.00 36.15 | CPS2 |
| MOTA | 1263 | C | LEU | 41 | 60.540 | 11.653 | 9.210 | 1.00 37.79 | CPS2 |
| ATOM | 1264 | 0 | LEU | 41 | 61.147 | 10.905 | 8.441 | 1.00 37.84 | CPS2 |
| MOTA | 1265 | N | SER | 42 | 59.231 | 11.882 | 9.130 | 1.00 38.99 | CPS2 |
| MOTA | 1266 | CA | SER | 42 | 58.394 | 11.272 | 8.105 | 1.00 39.66 | CPS2 |
| ATOM | 1267 | CB | SER | 42 | 56.916 | 11.461 | 8.451 | 1.00 40.41 | CPS2 |
| ATOM | 1268 | OG | SER | 42 | 56.529 | 12.813 | 8.277 | 1.00 40.55 | CPS2 |
| MOTA | 1269 | C | SER | 42 | 58.688 | 11.947 | 6.769 | 1.00 40.88 | CPS2 |
| ATOM | 1270 | 0 | SER | 42 | 59.404 | 12.948 | 6.716 | 1.00 40.22 | CPS2 |
| ATOM | 1271 | N | GLU | 43 | 58.118 | 11.405 | 5.698 | 1.00 41.38 | CPS2 |
| MOTA | 1272 | CA | GLU | 43 | 58.310 | 11.948 | 4.358 | 1.00 41.99 | CPS2 |
| MOTA | 1273 | CB | GLU | 43 | 57.466 | 11.173 | 3.340 | 1.00 44.33 | CPS2 |
| MOTA | 1274 | CG | GLU | 43 | 56.922 | 9.822 | 3.821 | 1.00 47.83 | CPS2 |
| MOTA | 1275 | CD | GLU | 43 | 55.963 | 9.946 | 5.005 | 1.00 50.30 | CPS2 |
| MOTA | 1276 | OE1 | GLU | 43 | 55.186 | 10.935 | 5.055 | 1.00 50.62 | CPS2 |
| ATOM | 1277 | OE2 | GLU | 43 | 55.982 | 9.045 | 5.877 | 1.00 48.97 | CPS2 |
| ATOM | 1278 | C | GLU | 43 | 57.921 | 13.425 | 4.294 | 1.00 40.64 | CPS2 |
| MOTA | 1279 | 0 | GLU | 43 | 58.662 | 14.259 | 3.767 | 1.00 40.30 | CPS2 |
| ATOM | 1280 | N | LYS | 44 | 56.747 | 13.739 | 4.825 | 1.00 39.19 | CPS2 |
| MOTA | 1281 | CA | LYS | 44 | 56.249 | 15.112 | 4.821 | 1.00 39.31 | CPS2 |
| MOTA | 1282 | CB | LYS | 44 | 54.787 | 15.140 | 5.269 | 1.00 40.00 | CPS2 |
| MOTA | 1283 | CG | LYS | 44 | 54.112 | 16.491 | 5.107 | 1.00 42.53 | CPS2 |
| ATOM | 1284 | CD | LYS | 44 | 52.721 | 16.472 | 5.719 | 1.00 44.55 | CPS2 |
| MOTA | 1285 | CE | LYS | 44 | 52.031 | 17.817 | 5.592 | 1.00 45.48 | CPS2 |
| ATOM | 1286 | NZ | LYS | 44 | 50.783 | 17.861 | 6.406 | 1.00 47.64 | CPS2 |
| ATOM | 1287 | C | LYS | 44 | 57.075 | 16.023 | 5.732 | 1.00 38.50 | CPS2 |
| ATOM | 1288 | 0 | LYS | 44 | 57.446 | 17.136 | 5.345 | 1.00 38.08 | CPS2 |
| ATOM | 1289 | N | ARG | 45 | 57.345 | 15.554 | 6.947 | 1.00 36.81 | CPS2 |
| MOTA | 1290 | CA | ARG | 45 | 58.125 | 16.335 | 7.898 | 1.00 36.28 | CPS2 CPS2 |
| ATOM | 1291 | CB | ARG | 45 | 58.162 | 15.624 | 9.254 | 1.00 37.98 | CPS2 |
| ATOM | 1292 | CG | ARG | 45 | 56.911 | 15.843 | 10.106 | 1.00 41.93 1.00 45.38 | CPS2 |
| ATOM | 1293 | CD | ARG | 45 | 57.135 | 16.960 | 11.117 | | CPS2 |
| MOTA | 1294 | NE | ARG | 45 | 57.655 | 18.160 | 10.468 | 1.00 49.29 | CPS2 |
| MOTA | 1295 | CZ | ARG | 45 | 58.565 | 18.968 | 11.002 | 1.00 49.81 | CPS2 |
| MOTA | 1296 | | ARG | 45 | 59.064 | 18.714 | 12.206 | 1.00 51.08 | |
| ATOM | 1297 | | ARG | 45 | 58.993 | 20.022 | 10.323 | 1.00 50.35 1.00 34.46 | CPS2 CPS2 |
| MOTA | 1298 | C | ARG | 45 | 59.537 | 16.595 | 7.382 | 1.00 34.46 | CPS2 |
| MOTA | 1299 | 0 | ARG | 45 | 60.105 | 17.657 | 7.629 | 1.00 33.18 | CPS2 |
| ATOM | 1300 | N | LYS | 46 | 60.107 | 15.630 | 6.662 | 1.00 32.44 | CPS2 |
| MOTA | 1301 | CA | LYS | 46 | 61.444 | 15.814 | 6.110 5.295 | 1.00 32.32 | CPS2 |
| MOTA | 1302 | CB | LYS | 46 | 61.891 | 14.589 | 6.133 | 1.00 32.43 | CPS2 |
| ATOM | 1303 | CG | LYS | 46 | 62.375 | 13.419 | 5.245 | 1.00 34.31 | CPS2 |
| ATOM | 1304 | CD | LYS | 46 | 62.872 | 12.296 | | 1.00 34.31 | CPS2 |
| MOTA | 1305 | CE | LYS | 46 46 | 63.389 | 11.131 | 6.065 5.169 | 1.00 36.69 | CPS2 |
| ATOM | 1306 | NZ | LYS | 46 | 63.700 | 9.994 | 5.206 | 1.00 31.46 | CPS2 |
| ATOM | 1307 | C | LYS | 46 46 | 61.479 | 17.039 | 5.206 | 1.00 31.48 | CPS2 |
| ATOM | 1308 | O NT | LYS | 46 47 | 62.393 60.481 | 17.856 | 4.336 | | CPS2 |
| ATOM | 1309 | N | ASN | 47 | | 17.163 | 3.407 | | CPS2 |
| ATOM | 1310 | CA | ASN | 47 | 60.417 | 18.286 | 3.40/ | 1.00 31.10 | 0104 |

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| ATOM | 1311 | CB | ASN | 47 | 59.240 | 18.101 | 2.437 | 1.00 32.45 | CPS2 |
|--------------|--------------|----------|------------|------------|------------------|------------------|-----------------|--------------------------|--------------|
| MOTA | 1312 | CG | ASN | 47 | 59.080 | 19.269 | 1.470 | 1.00 34.97 | CPS2 |
| ATOM | 1313 | OD1 | ASN | 47 | 59.977 | 19.575 | 0.684 | 1.00 37.44 | CPS2 |
| MOTA | 1314 | ND2 | | 47 | 57.928 | 19.923 | 1.525 | 1.00 35.87 | CPS2 |
| MOTA | 1315 | С | ASN | 47 | 60.290 | 19,612 | 4.157 | 1.00 29.73 | CPS2 |
| ATOM | 1316 | 0 | ASN | 47 | 60.946 | 20.587 | 3.803 | 1.00 28.79 | CPS2 |
| MOTA | 1317 | N | GLU | 48 | 59.462 | 19.637 | 5.195 | 1.00 28.89 | CPS2 |
| ATOM | 1318 | CA | GLU | 48 | 59.265 | 20.853 | 5.984 | 1.00 29.80 | CPS2 |
| ATOM | 1319 | CB | GLU | 48 | 58.162 | 20.642 | 7.019 | 1.00 32.74 | CPS2 |
| ATOM | 1320 | CG | GLU | 48 | 56.837 | 20.225 | 6.424 | 1.00 37.62 | CPS2 |
| ATOM | 1321 | CD | GLU | 48 | 55.785 | 19.953 | 7.482 | 1.00 40.29 | CPS2 |
| ATOM | 1322 | | GLU | 48 | 54.683 | 19.506 | 7.113 | 1.00 41.90 | C⊋S2 |
| ATOM | 1323 | | GLU | 48 | 56.059 | 20.193 | 8.679 | 1.00 42.74 | CPS2 |
| ATOM | 1324 | С | GLU | 48 | 60.554 | 21.231 | 6.700 | 1.00 28.72 | CPS2 |
| ATOM | 1325 | 0 | GLU | 48 | 60.956 | 22.396 | 6.720 | 1.00 27.50 | CPS2 |
| ATOM | 1326 | N | PHE | 49 | 61.192 | 20.230 | 7.296 | 1.00 26.72 | CPS2 |
| ATOM | 1327 | CA | PHE | 49 | 62.432 | 20.433 | 8.023 | 1.00 26.17 | CPS2 |
| ATOM | 1328 | CB | PHE | 49 | 62.877 | 19.116 | 8.665 | 1.00 27.12 | CPS2 |
| MOTA | 1329 | CG | PHE | 49 | 64.186 | 19.205 | 9.397 | 1.00 26.24 | CPS2 |
| ATOM | 1330 | | PHE | 49 | 64.219 | 19.514 | 10.750 | 1.00 27.02 | CPS2 |
| ATOM | 1331 | | PHE | 49 | 65.385 | 18.967 | 8.734 | 1.00 28.35 1.00 27.13 | CPS2 CPS2 |
| ATOM ATOM | 1332 1333 | | PHE PHE | 49 49 | 65.429 66.603 | 19.578 19.030 | 11.436 9.411 | 1.00 27.13 | CPS2 |
| ATOM | 1334 | CZ | PHE | 49 | 66.615 | 19.336 | 10.770 | 1.00 27.13 | CPS2 |
| ATOM | 1335 | C | PHE | 49 | 63.522 | 20.935 | 7.091 | 1.00 24.61 | CPS2 |
| ATOM | 1336 | 0 | PHE | 49 | 64.208 | 21.907 | 7.390 | 1.00 24.60 | CPS2 |
| ATOM | 1337 | Ŋ | LEU | 50 | 63.685 | 20.266 | 5.957 | 1.00 23.67 | CPS2 |
| ATOM | 1338 | CA | LEU | 50 | 64.710 | 20.650 | 5.000 | 1.00 23.23 | CPS2 |
| ATOM | 1339 | CB | LEU | 50 | 64.763 | 19.626 | 3.862 | 1.00 24.17 | CPS2 |
| ATOM | 1340 | CG | LEU | 50 | 65.810 | 19.767 | 2.758 | 1.00 26.00 | CPS2 |
| ATOM | 1341 | | LEU | 50 | 67.217 | 19.817 | 3.351 | 1.00 25.89 | CPS2 |
| MOTA | 1342 | CD2 | LEU | 50 | 65.685 | 18.570 | 1.810 | 1.00 26.96 | CPS2 |
| ATOM | 1343 | Ç | LEU | 50 | 64.465 | 22.053 | 4.448 | 1.00 23.30 | CPS2 |
| MOTA | 1344 | 0 | LEU | 50 | 65.391 | 22.849 | 4.317 | 1.00 22.85 | CPS2 |
| MOTA | 1345 | N | ALA | 51 | 63.218 | 22.366 | 4.127 | 1.00 21.99 | CPS2 |
| ATOM | 1346 | CA | ALA | 51 | 62.914 | 23.684 | 3.586 | 1.00 21.37 | CPS2 |
| ATOM | 1347 | CB | ALA | 51 | 61.438 | 23.766 | 3.206 | 1.00 19.49 | CPS2 |
| ATOM | 1348 | С | ALA | 51 | 63.262 | 24.772 | 4.610 | 1.00 19.95 | CPS2 |
| ATOM | 1349 | 0 | ALA | 51 | 63.812 | 25.815 | 4.252 | 1.00 19.91 | CPS2 |
| ATOM | 1350 | N | GLY | 52 | 62.943 | 24.508 | 5.871 | 1.00 20.32 | CPS2 |
| ATOM | 1351 | CA | GLY | 52 | 63.207 | 25.466 | 6.939 | 1.00 20.53 | CPS2 |
| ATOM | 1352 | C | GLY | 52 | 64.690 | 25.678 | 7.161 | 1.00 21.59 | CPS2 |
| ATOM | 1353 | 0 | GLY | 52 | 65.140 | 26.823 | 7.292 | 1.00 20.12 | CPS2 |
| ATOM | 1354 | N | ARG | 53 | 65.452 | 24.581 | 7.211 | 1.00 20.75 | CPS2 CPS2 |
| ATOM | 1355 | CA | ARG | 53 53 | 66.900 | 24.681 | 7.405 | 1.00 21.49 1.00 20.94 | CPS2 |
| MOTA | 1356 | CB | ARG | 53 | 67.511 | 23.289 | 7.639 | 1.00 20.94 | CPS2 |
| MOTA | 1357 | CG | ARG | 53 53 | 67.662 | 22.904 | 9.121 9.905 | 1.00 23.39 | CPS2 |
| ATOM | 1358 | CD | ARG | 53 53 | 66.357 | 23.082 | 11.335 | 1.00 24.30 | CPS2 |
| ATOM | 1359 | NE CZ | ARG ARG | 53 53 | 66.538 65.666 | 22.829 23.195 | 12.272 | 1.00 25.08 | CPS2 |
| ATOM | 1360 1361 | | ARG | 53 53 | 64.548 | 23.193 | 11.934 | 1.00 25.43 | CPS2 |
| ATOM ATOM | 1362 | | ARG | 53 53 | 65.921 | 22.959 | 13.551 | 1.00 26.80 | CPS2 |
| ATOM | 1363 | C | ARG | 53 53 | 67.541 | 25.359 | 6.201 | 1.00 20.90 | CPS2 |
| ATOM | 1364 | 0 | ARG | 53 | 68.447 | 26.176 | 6.353 | 1.00 20.27 | CPS2 |
| ATOM | 1365 | N | PHE | 5 4 | 67.069 | 25.021 | 5.002 | 1.00 20.29 | CPS2 |
| ATOM | 1366 | CA | PHE | 54 | 67.583 | 25.631 | 3.779 | 1.00 21.05 | CPS2 |
| ATOM | 1367 | CB | PHE | 54 | 66.889 | 24.996 | 2.550 | 1.00 21.38 | CPS2 |
| ATOM | 4307 | رن | | J-1 | J | ٥٠٠٠ | | | |

| MOTA | 1368 | CG | PHE | 54 | 67.310 | 25.573 | 1.218 | 1.00 22.85 | CPS2 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| ATOM | 1369 | CD1 | PHE | 54 | 66.623 | 25.646 | 0.660 | 1.00 23.51 | CPS2 |
| ATOM | 1370 | CD2 | PHE | 54 | 68.363 | 25.008 | 0.495 | 1.00 23.11 | CPS2 |
| MOTA | 1371 | CEl | PHE | 54 | 66.970 | 27.148 | -0.600 | 1.00 23.62 | CPS2 |
| MOTA | 1372 | CE2 | PHE | 54 | 68.716 | 25.499 | -0.761 | 1.00 24.74 | CPS2 |
| ATOM | 1373 | CZ | PHE | 54 | 68.015 | 26.575 | -1.313 | 1.00 24.84 | CPS2 |
| ATOM | 1374 | C | PHE | 54 | 67.334 | 27.144 | 3.823 | 1.00 20.71 | CPS2 |
| MOTA | 1375 | 0 | PHE | 54 | 68.225 | 27.939 | 3.523 | 1.00 20.44 | CPS2 |
| MOTA | 1376 | N | ALA | 55 | 66.118 | 27.542 | 4.191 | 1.00 20.38 | CPS2 |
| ATOM | 1377 | CA | ALA | 55 | 65.772 | 28.967 | 4.268 | 1.00 20.18 | CPS2 |
| ATOM | 1378 | CB | ALA | 55 | 64.299 | 29.138 | 4.665 | 1.00 19.50 | CPS2 |
| ATOM | 1379 | С | ALA | 55 | 66.654 | 29.701 | 5.276 | 1.00 20.15 | CPS2 |
| ATOM | 1380 | 0 | ALA | 55 | 67.111 | 30.822 | 5.021 | 1.00 19.68 | CPS2 |
| ATOM | 1381 | N | ALA | 56 | 66.872 | 29.071 | 6.428 | 1.00 20.22 | CPS2 |
| ATOM | 1382 | CA | ALA | 56 | 67.706 | 29.657 | 7.476 | 1.00 19.63 | CPS2 |
| ATOM | 1383 | CB | ALA | 56 | 67.670 | 28.772 | 8.737 | 1.00 20.93 | CPS2 |
| ATOM | 1384 | C | ALA | 56 | 69.152 | 29.841 | 7.014 | 1.00 20.43 | CPS2 |
| ATOM | 1385 | 0 | ALA | 56 | 69.780 | 30.869 | 7.307 | 1.00 19.00 | CPS2 |
| ATOM | 1386 | N | LYS | 57 | 69.702 | 28.840 | 6.322 | 1.00 19.36 | CPS2 |
| ATOM | 1387 | CA | LYS | 57 | 71.084 | 28.955 | 5.858 | 1.00 19.89 | CPS2 |
| ATOM | 1388 | CB | LYS | 57 | 71.622 | 27.598 | 5.388 | 1.00 19.91 | CPS2 |
| ATOM | 1389 | CG | LYS | 57 | 71.595 | 26.550 | 6.501 | 1.00 20.56 | CFS2 |
| ATOM | 1390 | CD | LYS | 57 | 72.389 | 25.285 | 6.150 | 1.00 21.63 | CPS2 |
| ATOM | 1391 | CE | LYS | 57 | 72.426 | 24.334 | 7.358 | 1.00 20.15 | CPS2 |
| MOTA | 1392 | NZ | LYS | 57 | 73.457 | 23.262 | 7.208 | 1.00 19.99 | CPS2 |
| ATOM | 1393 | C | LYS | 57 | 71.176 | 29.993 | 4.754 | 1.00 19.82 | CPS2 |
| MOTA | 1394 | 0 | LYS | 57 | 72.136 | 30.755 | 4.698 | 1.00 20.57 | CPS2 |
| ATOM | 1395 | N | GLU | 58 | 70.179 | 30.036 | 3.871 | 1.00 18.71 | CPS2 |
| ATOM | 1396 | CA | GLU | 58 | 70.187 | 31.045 | 2.822 | 1.00 20.25 | CPS2 |
| MOTA | 1397 | CB | GLU | 58 | 68.993 | 30.868 | 1.870 | 1.00 23.44 | CPS2 |
| ATOM | 1398 | CG | GLU | 58 | 69.120 | 29.710 | 0.871 | 1.00 28.15 | CPS2 |
| ATOM | 1399 | CD | GLU | 58 | 70.251 | 29.896 | -0.124 | 1.00 31.42 | CPS2 |
| ATOM | 1400 | | GLU | 58 | 70.713 | 31.042 | -0.335 | 1.00 33.78 | CPS2 |
| MOTA | 1401 | | GLU | 58 | 70.701 | 28.891 | -0.713 | 1.00 35.13 | CPS2 |
| ATOM | 1402 | C | GLU | 58 | 70.116 | 32.436 | 3.477 | 1.00 20.06 | CPS2 |
| MOTA | 1403 | 0 | GLU | 58 | 70.878 | 33.335 | 3.117 | 1.00 20.02 | CPS2 |
| MOTA | 1404 | N | ALA | 59 | 69.203 | 32.611 | 4.433 | 1.00 18.56 | CPS2 |
| ATOM | 1405 | CA | ALA | 59 | 69.066 | 33.901 | 5.107 | 1.00 19.36 | CPS2 |
| ATOM | 1406 | CB | ALA | 59 | 67.919 | 33.853 | 6.142 | 1.00 18.28 | CPS2 |
| ATOM | 1407 | С | ALA | 59 | 70.388 | 34.280 | 5.789 | 1.00 19.60 | CPS2 |
| ATOM | 1408 | 0 | ALA | 59 | 70.833 | 35.429 | 5.712 | 1.00 20.42 | CPS2 |
| ATOM | 1409 | N | PHE | 60 | 71.016 | 33.314 | 6.452 | 1.00 18.99 | CPS2 |
| MOTA | 1410 | CA | PHE | 60 | 72.284 | 33.591 | 7.119 | 1.00 19.29 | CPS2 |
| ATOM | 1411 | CB | PHE | 60 | 72.790 | 32.350 | 7.862 | 1.00 20.46 | CPS2 |
| ATOM | 1412 | CG | PHE | 60 | 74.128 | 32.555 | 8.501 | 1.00 21.05 | CPS2 |
| MOTA | 1413 | CD1 | PHE | 60 | 74.225 | 33.085 | 9.785 | 1.00 21.57 | CPS2 |
| ATOM | 1414 | | PHE | 60 | 75.297 | 32.313 | 7.783 | 1.00 23.12 | CPS2 |
| ATOM | 1415 | | PHE | 60 | 75.476 | 33.377 | 10.343 | 1.00 22.68 | CPS2 |
| MOTA | 1416 | | PHE | 60 | 76.554 | 32.605 | 8.332 | 1.00 22.55 | CPS2 |
| ATOM | 1417 | CZ | PHE | 60 | 76.638 | 33.136 | 9.610 | 1.00 22.82 | CPS2 |
| ATOM | 1418 | C | PHE | 60 | 73.338 | 34.020 | 6.092 | 1.00 20.21 | CPS2 |
| ATOM | 1419 | 0 | PHE | 60 | 74.089 | 34.965 | 6.320 | 1.00 19.97 | CPS2 |
| ATOM | 1420 | N | SER | 61 | 73.396 | 33.318 | 4.960 | 1.00 20.80 | CPS2 |
| ATOM | 1421 | CA | SER | 61 | 74.372 | 33.641 | 3.920 | 1.00 20.87 | CPS2 |
| MOTA | 1422 | CB | SER | 61 | 74.287 | 32.633 | 2.762 | 1.00 21.27 | CPS2 |
| MOTA | 1423 | OG | SER | 61 | 73.161 | 32.874 | 1.942 | 1.00 22.46 | CPS2 |
| ATOM | 1424 | C | SER | 61 | 74.190 | 35.058 | 3.389 | 1.00 21.75 | CPS2 |
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| ATOM | 1425 | 0 | SER | 61 | 75.161 | 35.709 | 2.981 | 1.00 22.83 | CPS2 |
|------|------|-----|-----|----|--------|--------|--------|--------------------------|--------------|
| ATOM | 1426 | N | LYS | 62 | 72.949 | 35.541 | 3.396 | 1.00 20.78 | CPS2 |
| ATOM | 1427 | CA | LYS | 62 | 72.657 | 36.890 | 2.934 | 1.00 21.54 | CPS2 |
| ATOM | 1428 | CB | LYS | 62 | 71.158 | 37.027 | 2.627 | 1.00 22.99 | CPS2 |
| ATOM | 1429 | CG | LYS | 62 | 70.696 | 36.164 | 1.444 | 1.00 27.37 | CPS2 |
| MOTA | 1430 | CD | LYS | 62 | 69.195 | 35.912 | 1.505 | 1.00 30.44 | CPS2 |
| ATOM | 1431 | CE | LYS | 62 | 68.439 | 36.617 | 0.401 | 1.00 33.74 | CPS2 |
| ATOM | 1432 | NZ | LYS | 62 | 68.581 | 35.960 | -0.917 | 1.00 35.02 | CPS2 |
| MOTA | 1433 | C | LYS | 62 | 73.084 | 37.922 | 3.985 | 1.00 22.13 | CPS2 |
| MOTA | 1434 | 0 | LYS | 62 | 73.546 | 39.009 | 3.638 | 1.00 22.23 | CPS2 |
| MOTA | 1435 | N | ALA | 63 | 72.929 | 37.581 | 5.264 | 1.00 21.23 | CPS2 |
| ATOM | 1436 | CA | ALA | 63 | 73.329 | 38.488 | 6.335 | 1.00 20.30 | CPS2 |
| ATOM | 1437 | CB | ALA | 63 | 72.813 | 37.988 | 7.694 | 1.00 21.99 | CPS2 |
| MOTA | 1438 | С | ALA | 63 | 74.851 | 38.541 | 6.337 | 1.00 22.63 | CPS2 |
| ATOM | 1439 | 0 | ALA | 63 | 75.439 | 39.604 | 6.541 | 1.00 22.47 | CPS2 |
| ATOM | 1440 | N | PHE | 64 | 75.473 | 37.387 | 6.092 | 1.00 23.43 | CPS2 |
| MOTA | 1441 | CA | PHE | 64 | 76.934 | 37.257 | 6.040 | 1.00 26.03 | CPS2 |
| ATOM | 1442 | CB | PHE | 64 | 77.315 | 35.788 | 5.814 | 1.00 28.19 | CPS2 |
| MOTA | 1443 | CG | PHE | 64 | 78.780 | 35.482 | 6.042 | 1.00 31.14 | CPS2 |
| ATOM | 1444 | CD1 | PHE | 64 | 79.301 | 35.418 | 7.329 | 1.00 33.14 | CPS2 |
| ATOM | 1445 | CD2 | PHE | 64 | 79.624 | 35.224 | 4.965 | 1.00 32.47 | CPS2 |
| MOTA | 1446 | CE1 | PHE | 64 | 80.652 | 35.094 | 7.545 | 1.00 34.43 | CPS2 |
| MOTA | 1447 | CE2 | PHE | 64 | 80.969 | 34.900 | 5.163 | 1.00 33.63 | CPS2 |
| ATOM | 1448 | CZ | PHE | 64 | 81.484 | 34.834 | 6.457 | 1.00 33.53 | CPS2 |
| ATOM | 1449 | C | PHE | 64 | 77.481 | 38.136 | 4.905 | 1.00 27.97 | CPS2 |
| MOTA | 1450 | 0 | PHE | 64 | 78.645 | 38.549 | 4.935 | 1.00 29.10 | CPS2 |
| MOTA | 1451 | N | GLY | 65 | 76.642 | 38.388 | 3.901 | 1.00 28.14 | CPS2 |
| ATOM | 1452 | CA | GLY | 65 | 76.999 | 39.256 | 2.786 | 1.00 29.01 | CPS2 |
| ATOM | 1453 | С | GLY | 65 | 77.588 | 38.652 | 1.523 | 1.00 30.18 | CPS2 |
| ATOM | 1454 | 0 | GLY | 65 | 77.945 | 39.377 | 0.596 | 1.00 31.12 | CPS2 |
| ATOM | 1455 | N | THR | 66 | 77.660 | 37.332 | 1.454 | 1.00 30.26 | CPS2 |
| MOTA | 1456 | CA | THR | 66 | 78.268 | 36.684 | 0.302 | 1.00 30.90 | CPS2 |
| ATOM | 1457 | CB | THR | 66 | 79.499 | 35.898 | 0.744 | 1.00 30.61 | CPS2 |
| MOTA | 1458 | OG1 | | 66 | 79.078 | 34.838 | 1.507 | 1.00 32.42 | CPS2 |
| MOTA | 1459 | | THR | 66 | 80.457 | 36.790 | 1.525 | 1.00 31.71 | CPS2 |
| ATOM | 1460 | C | THR | 66 | 77.362 | 35.697 | -0.410 | 1.00 31.06 | CPS2 |
| ATOM | 1461 | 0 | THR | 66 | 77.601 | 35.355 | -1.573 | 1.00 32.11 | CPS2 |
| ATOM | 1462 | N | GLY | 67 | 76.332 | 35.232 | 0.288 | 1.00 30.08 | CPS2 |
| ATOM | 1463 | CA | GLY | 67 | 75.460 | 34.226 | -0.285 | 1.00 29.32 | CPS2 |
| MOTA | 1464 | C | GLY | 67 | 76.230 | 32.923 | -0.146 | 1.00 29.07 | CPS2 |
| ATOM | 1465 | 0 | GLY | 67 | 77.357 | 32.929 | 0.354 | 1.00 28.18 | CPS2 |
| MOTA | 1466 | N | ILE | 68 | 75.640 | 31.809 | -0.566 | 1.00 29.24 | CPS2 |
| MOTA | 1467 | CA | ILE | 68 | 76.315 | 30.518 | -0.477 | 1.00 30.11 | CPS2 |
| MOTA | 1468 | CB | ILE | 68 | 75.293 | 29.347 | -0.467 | 1.00 29.33 | CPS2 |
| MOTA | 1469 | | ILE | 68 | 76.018 | 28.010 | -0.446 | 1.00 29.51 | CPS2 |
| ATOM | 1470 | | ILE | 68 | 74.388 | 29.434 | 0.769 | 1.00 28.22 | CPS2 |
| ATOM | 1471 | | ILE | 68 | 75.100 | 29.195 | 2.089 | 1.00 25.10 | CPS2 |
| MOTA | 1472 | С | ILE | 68 | 77.237 | 30.385 | -1.697 | 1.00 32.39 | CPS2 |
| ATOM | 1473 | 0 | ILE | 68 | 76.831 | 30.654 | -2.827 | 1.00 32.91 | CPS2 |
| ATOM | 1474 | N | GLY | 69 | 78.476 | 29.979 | -1.460 | 1.00 32.97 | CPS2 |
| ATOM | 1475 | CA | GLY | 69 | 79.419 | 29.834 | -2.552 | 1.00 35.33 | CPS2 |
| ATOM | 1476 | C | GLY | 69 | 80.810 | 29.564 | -2.028 | 1.00 36.14 | CPS2 |
| MOTA | 1477 | 0 | GLY | 69 | 80.970 | 28.924 | -0.992 | 1.00 36.01 | CPS2 |
| ATOM | 1478 | N | ALA | 70 | 81.814 | 30.065 | -2.742 | 1.00 37.62 | CPS2 |
| ATOM | 1479 | CA | ALA | 70 | 83.212 | 29.872 | -2.379 | 1.00 38.31 | CPS2 CPS2 |
| ATOM | 1480 | CB | ALA | 70 | 84.110 | 30.468 | -3.473 | 1.00 38.64 1.00 38.65 | CPS2 |
| MOTA | 1481 | С | ALA | 70 | 83.577 | 30.474 | -1.025 | 1.00 30.03 | CESS |
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| 3.5004 | | _ | | | | | | | |
|--------|------|-----|-----|------------|--------|--------|--------|------------|------|
| MOTA | 1482 | 0 | ALA | 70 | 84.488 | 29.999 | -0.345 | 1.00 39.72 | CPS2 |
| MOTA | 1483 | И | GLN | 71 | 82.858 | 31.515 | -0.628 | 1.00 38.67 | CPS2 |
| ATOM | 1484 | CA | GLN | 71 | 83.130 | 32.197 | 0.630 | 1.00 37.32 | CPS2 |
| ATOM | 1485 | CB | GLN | 71 | 82.744 | 33.666 | 0.472 | 1.00 40.43 | CPS2 |
| ATOM | 1486 | CG | GLN | 71 | 83.693 | 34.659 | 1.118 | 1.00 44.57 | CPS2 |
| ATOM | 1487 | CD | GLN | 71 | 83.654 | 36.018 | 0.431 | 1.00 46.06 | CPS2 |
| ATOM | 1488 | OE1 | | 71 | 84.175 | 37.004 | 0.952 | 1.00 48.20 | |
| | | | | | | | | | CPS2 |
| ATOM | 1489 | NE2 | | 71 | 83.044 | 36.069 | -0.754 | 1.00 47.40 | CPS2 |
| MOTA | 1490 | C | GLN | 71 | 82.391 | 31.578 | 1.824 | 1.00 35.81 | CPS2 |
| MOTA | 1491 | 0 | GLN | 71 | 82.851 | 31.656 | 2.962 | 1.00 36.15 | CPS2 |
| MOTĄ | 1492 | N | LEU | 72 | 81.257 | 30.944 | 1.561 | 1.00 32.57 | CPS2 |
| ATOM | 1493 | CA | LEU | 72 | 80.461 | 30.353 | 2.630 | 1.00 30.34 | CPS2 |
| ATOM | 1494 | CB | LEU | 72 | 79.503 | 31.400 | 3.196 | 1.00 29.93 | CPS2 |
| ATOM | 1495 | CG | LEU | 72 | 78.560 | 30.935 | 4.303 | 1.00 29.85 | CPS2 |
| ATOM | 1496 | | LEU | 72 | 79.352 | 30.712 | 5.585 | 1.00 29.87 | CPS2 |
| ATOM | 1497 | | LEU | 72 | | | | | |
| | | | | | 77.482 | 31.998 | 4.515 | 1.00 30.13 | CPS2 |
| ATOM | 1498 | С | LEU | 72 | 79.670 | 29.165 | 2.117 | 1.00 28.96 | CPS2 |
| MOTA | 1499 | 0 | LEU | 72 | 78.925 | 29.270 | 1.146 | 1.00 29.65 | CPS2 |
| ATOM | 1500 | N | SER | 73 | 79.828 | 28.037 | 2.791 | 1.00 26.89 | CPS2 |
| MOTA | 1501 | CA | SER | 73 | 79.163 | 26.805 | 2.405 | 1.00 26.28 | CPS2 |
| MOTA | 1502 | CB | SER | 73 | 80.176 | 25.656 | 2.498 | 1.00 27.70 | CPS2 |
| MOTA | 1503 | OG | SER | 73 | 79.571 | 24.385 | 2.324 | 1.00 31.43 | CPS2 |
| MOTA | 1504 | C | SER | 73 | 77.970 | 26.491 | 3.300 | 1.00 25.59 | CPS2 |
| MOTA | 1505 | ō | SER | 73 | 77.912 | 26.952 | 4.441 | 1.00 23.26 | CPS2 |
| ATOM | 1506 | N | PHE | 74 | 77.016 | 25.718 | 2.780 | 1.00 24.61 | CPS2 |
| ATOM | 1507 | CA | PHE | 74 | 75.874 | 25.292 | 3.591 | 1.00 24.31 | CPS2 |
| | | | | | | | | | |
| ATOM | 1508 | CB | PHE | 74 | 74.974 | 24.333 | 2.813 | 1.00 24.91 | CPS2 |
| ATOM | 1509 | CG | PHE | 74 | 74.016 | 25.012 | 1.887 | 1.00 27.32 | CPS2 |
| ATOM | 1510 | | PHE | 74 | 73.041 | 25.873 | 2.385 | 1.00 26.95 | CPS2 |
| ATOM | 1511 | | PHE | 74 | 74.079 | 24.787 | 0.511 | 1.00 28.10 | CPS2 |
| ATOM | 1512 | CE1 | PHE | 74 | 72.142 | 26.501 | 1.528 | 1.00 28.03 | CPS2 |
| MOTA | 1513 | CE2 | PHE | 74 | 73.185 | 25.411 | -0.350 | 1.00 29.15 | CPS2 |
| MOTA | 1514 | CZ | PHE | 74 | 72.214 | 26.271 | 0.160 | 1.00 27.71 | CPS2 |
| MOTA | 1515 | C | PHE | 74 | 76.433 | 24.527 | 4.788 | 1.00 25.14 | CPS2 |
| ATOM | 1516 | 0 | PHE | 74 | 75.841 | 24.490 | 5.868 | 1.00 23.71 | CPS2 |
| ATOM | 1517 | N | GLN | 75 | 77.577 | 23.886 | 4.571 | 1.00 25.35 | CPS2 |
| ATOM | 1518 | CA | GLN | 75 | 78.212 | 23.099 | 5.618 | 1.00 26.61 | CPS2 |
| ATOM | 1519 | CB | GLN | 75 | 79.212 | 22.115 | 4.998 | 1.00 26.65 | CPS2 |
| | | | | | 78.580 | | | 1.00 27.20 | CPS2 |
| ATOM | 1520 | CG | GLN | 75 75 | | 21.089 | 4.063 | | |
| ATOM | 1521 | CD | GLN | 75 | 77.513 | 20.259 | 4.742 | 1.00 26.33 | CPS2 |
| ATOM | 1522 | OE1 | | 75 | 77.695 | 19.797 | 5.864 | 1.00 26.93 | CPS2 |
| ATOM | 1523 | NE2 | | 75 | 76.390 | 20.057 | 4.056 | 1.00 27.72 | CPS2 |
| ATOM | 1524 | C | GLN | 75 | 78.918 | 23.944 | 6.674 | 1.00 27.33 | CPS2 |
| MOTA | 1525 | 0 | GLN | 75 | 79.380 | 23.413 | 7.684 | 1.00 30.23 | CPS2 |
| MOTA | 1526 | N | ASP | 76 | 79.020 | 25.250 | 6.455 | 1.00 28.01 | CPS2 |
| MOTA | 1527 | CA | ASP | 76 | 79.676 | 26.113 | 7.441 | 1.00 26.83 | CPS2 |
| ATOM | 1528 | CB | ASP | 76 | 80.334 | 27.317 | 6.769 | 1.00 28.17 | CPS2 |
| ATOM | 1529 | CG | ASP | 76 | 81.508 | 26.933 | 5.900 | 1.00 29.80 | CPS2 |
| ATOM | 1530 | | ASP | 76 | 82.291 | 26.066 | 6.330 | 1.00 29.26 | CPS2 |
| | | | | | | | 4.800 | 1.00 30.74 | CPS2 |
| ATOM | 1531 | | ASP | 76 76 | 81.649 | 27.514 | | | CPS2 |
| ATOM | 1532 | C | ASP | 76 | 78.657 | 26.648 | 8.429 | 1.00 27.59 | |
| ATOM | 1533 | 0 | ASP | 76 | 79.015 | 27.306 | 9.412 | 1.00 26.97 | CPS2 |
| ATOM | 1534 | N | ILE | 7 7 | 77.389 | 26.352 | 8.164 | 1.00 26.05 | CPS2 |
| ATOM | 1535 | CA | ILE | 7 7 | 76.280 | 26.859 | 8.970 | 1.00 25.04 | CPS2 |
| MOTA | 1536 | CB | ILE | 77 | 75.306 | 27.678 | 8.079 | 1.00 23.67 | CPS2 |
| MOTA | 1537 | CG2 | ILE | 77 | 74.270 | 28.414 | 8.942 | 1.00 24.94 | CPS2 |
| MOTA | 1538 | | ILE | 7 7 | 76.085 | 28.674 | 7.218 | 1.00 23.77 | CPS2 |
| | | | | | | | | | |

| ATOM | 1539 | CD1 | ILE | 77 | 75.276 | 29.187 | 6.019 | 1.00 23.94 | CPS2 |
|------|------|-----|-----|----------|--------|--------|--------|------------|-------|
| ATOM | 1540 | C | ILE | 77 | 75.487 | 25.717 | 9.586 | 1.00 25.85 | CPS2 |
| ATOM | 1541 | 0 | ILE | 77 | 75.077 | 24.796 | 8.887 | 1.00 26.62 | CPS2 |
| ATOM | 1542 | N | GLU | 78 | 75.260 | 25.773 | 10.892 | 1.00 24.57 | CP\$2 |
| ATOM | 1543 | CA | GLU | 78 | 74.483 | 24.727 | 11.529 | 1.00 24.12 | CPS2 |
| ATOM | 1544 | CB | GLU | 78 | 75.366 | 23.875 | 12.450 | 1.00 24.96 | CPS2 |
| ATOM | 1545 | CG | GLU | 78 | 74.631 | 22.661 | 13.039 | 1.00 24.30 | CPS2 |
| ATOM | 1546 | CD | GLU | 78 | 75.579 | 21.638 | 13.643 | 1.00 30.06 | CPS2 |
| MOTA | 1547 | OE1 | | 78 | 75.989 | 21.815 | 14.805 | | |
| ATOM | 1548 | OE2 | | 78 | 75.930 | 20.656 | | 1.00 30.41 | CPS2 |
| ATOM | 1549 | C | GLU | 78 | | 25.285 | 12.942 | 1.00 30.57 | CPS2 |
| | | | | | 73.314 | | 12.326 | 1.00 25.19 | CPS2 |
| ATOM | 1550 | 0 | GLU | 78 | 73.467 | 26.243 | 13.096 | 1.00 24.62 | CPS2 |
| ATOM | 1551 | N | ILE | 79 70 | 72.139 | 24.697 | 12.124 | 1.00 23.01 | CPS2 |
| ATOM | 1552 | CA | ILE | 79 | 70.969 | 25.113 | 12.866 | 1.00 22.64 | CPS2 |
| ATOM | 1553 | CB | ILE | 79 | 69.673 | 25.081 | 12.014 | 1.00 23.46 | CPS2 |
| ATOM | 1554 | CG2 | | 79 | 68.519 | 25.648 | 12.832 | 1.00 25.86 | CPS2 |
| ATOM | 1555 | CG1 | | 79 | 69.868 | 25.835 | 10.688 | 1.00 25.21 | CPS2 |
| MOTA | 1556 | CD1 | | 79 | 70.337 | 27.256 | 10.820 | 1.00 27.02 | CPS2 |
| MOTA | 1557 | C | ILE | 79 | 70.832 | 24.078 | 13.970 | 1.00 23.01 | CPS2 |
| MOTA | 1558 | 0 | ILE | 79 | 70.679 | 22.882 | 13.691 | 1.00 22.93 | CPS2 |
| MOTA | 1559 | И | ARG | 80 | 70.912 | 24.524 | 15.217 | 1.00 21.65 | CPS2 |
| MOTA | 1560 | CA | ARG | 80 | 70.765 | 23.624 | 16.348 | 1.00 23.25 | CPS2 |
| MOTA | 1561 | CB | ARG | 80 | 71.928 | 23.793 | 17.322 | 1.00 22.55 | CPS2 |
| ATOM | 1562 | CG | ARG | 80 | 73.275 | 23.474 | 16.692 | 1.00 22.62 | CPS2 |
| MOTA | 1563 | CD | ARG | 80 | 74.373 | 23.461 | 17.742 | 1.00 22.35 | CPS2 |
| MOTA | 1564 | NE | ARG | 80 | 75.680 | 23.201 | 17.147 | 1.00 21.40 | CPS2 |
| ATOM | 1565 | CZ | ARG | 80 | 76.820 | 23.280 | 17.823 | 1.00 22.68 | CPS2 |
| MOTA | 1566 | NHl | ARG | 80 | 76.802 | 23.614 | 19.110 | 1.00 20.04 | CPS2 |
| MOTA | 1567 | NH2 | ARG | 80 | 77.971 | 23.020 | 17.216 | 1.00 22.34 | CPS2 |
| MOTA | 1568 | С | ARG | 80 | 69.456 | 23.947 | 17.044 | 1.00 24.16 | CPS2 |
| MOTA | 1569 | 0 | ARG | 80 | 68.837 | 24.965 | 16.757 | 1.00 23.92 | CPS2 |
| MOTA | 1570 | N | LYS | 81 | 69.028 | 23.074 | 17.947 | 1.00 26.40 | CPS2 |
| MOTA | 1571 | CA | LYS | 81 | 67.789 | 23.290 | 18.684 | 1.00 27.93 | CPS2 |
| MOTA | 1572 | CB | LYS | 81 | 66.840 | 22.108 | 18.466 | 1.00 30.60 | CPS2 |
| ATOM | 1573 | CG | LYS | 81 | 66.517 | 21.865 | 17.000 | 1.00 32.31 | CPS2 |
| ATOM | 1574 | CD | LYS | 81 | 65.759 | 20.561 | 16.767 | 1.00 36.54 | CPS2 |
| ATOM | 1575 | CE | LYS | 81 | 64.326 | 20.645 | 17.248 | 1.00 39.00 | CPS2 |
| ATOM | 1576 | NZ | LYS | 81 | 63.553 | 19.423 | 16.848 | 1.00 41.89 | CPS2 |
| ATOM | 1577 | C | LYS | 81 | 68.113 | 23.428 | 20.168 | 1.00 28.77 | CPS2 |
| ATOM | 1578 | 0 | LYS | 81 | 68.933 | 22.671 | 20.696 | 1.00 28.58 | CPS2 |
| ATOM | 1579 | N | ASP | 82 | 67.487 | 24.391 | 20.837 | 1.00 27.27 | CPS2 |
| ATOM | 1580 | CA | ASP | 82 | 67.741 | 24.576 | 22.258 | 1.00 29.97 | CPS2 |
| MOTA | 1581 | CB | ASP | 82 | 67.521 | 26.039 | 22.666 | 1.00 28.54 | CPS2 |
| MOTA | 1582 | CG | | 82 | 66.074 | 26.488 | 22.541 | 1.00 30.11 | CPS2 |
| MOTA | 1583 | | ASP | 82 | 65.846 | 27.715 | 22.575 | 1.00 28.52 | CPS2 |
| ATOM | 1584 | | ASP | 82 | 65.170 | 25.633 | 22.424 | 1.00 30.87 | CPS2 |
| ATOM | 1585 | C | ASP | 82 | 66.887 | 23.619 | 23.095 | 1.00 30.91 | CPS2 |
| | 1586 | 0 | ASP | 82 | 66.268 | 22.707 | 22.546 | 1.00 30.68 | CPS2 |
| ATOM | | | GLN | 83 | 66.867 | 23.819 | 24.411 | 1.00 33.59 | CPS2 |
| ATOM | 1587 | N | GLN | 83 | 66.120 | 22.941 | 25.313 | 1.00 36.28 | CPS2 |
| ATOM | 1588 | CA | | | | 23.356 | 26.772 | 1.00 37.73 | CPS2 |
| ATOM | 1589 | CB | GLN | 83 | 66.334 | 24.608 | | 1.00 37.73 | CPS2 |
| ATOM | 1590 | CG | GLN | 83 | 65.575 | | 27.198 | 1.00 41.41 | CPS2 |
| ATOM | 1591 | CD | GLN | 83 | 66.435 | 25.862 | 27.228 | 1.00 44.27 | CPS2 |
| MOTA | 1592 | | GLN | 83 | 66.892 | 26.355 | 26.187 | | CPS2 |
| MOTA | 1593 | | GLN | 83 | 66.659 | 26.389 | 28.432 | 1.00 43.27 | CPS2 |
| MOTA | 1594 | C | GLN | 83 | 64.626 | 22.892 | 25.022 | 1.00 37.29 | |
| MOTA | 1595 | 0 | GLN | 83 | 63.943 | 21.933 | 25.398 | 1.00 38.48 | CPS2 |

| MOTA | 1596 | N | ASN | 84 | 64.120 | 23.927 | 24.362 | 1.00 36.62 | CPS2 |
|--------|------|-----|-----|-----|--------|--------|--------|------------|------|
| MOTA | 1597 | CA | ASN | 84 | 62.707 | 23.996 | 24.024 | 1.00 36.63 | CPS2 |
| MOTA | 1598 | CB | ASN | 84 | 62.168 | 25.389 | 24.347 | 1.00 37.40 | CPS2 |
| MOTA | 1599 | CG | ASN | 84 | 62.263 | 25.716 | 25.828 | 1.00 38.82 | CPS2 |
| ATOM | 1600 | OD1 | ASN | 84 | 61.807 | 24.945 | 26.675 | 1.00 39.51 | CPS2 |
| ATOM | 1601 | ND2 | ASN | 84 | 62.856 | 26.857 | 26.148 | 1.00 38.34 | CPS2 |
| ATOM | 1602 | С | ASN | 84 | 62.456 | 23.661 | 22.556 | 1.00 36.23 | CPS2 |
| ATOM | 1603 | o | ASN | 84 | 61.345 | 23.839 | 22.052 | | |
| | | | | | | | | 1.00 36.16 | CPS2 |
| ATOM | 1604 | N | GLY | 85 | 63.492 | 23.173 | 21.879 | 1.00 34.68 | CPS2 |
| ATOM | 1605 | CA | GLY | 85 | 63.370 | 22.814 | 20.476 | 1.00 33.60 | CPS2 |
| ATOM | 1606 | C | GLY | 85 | 63.425 | 23.999 | 19.523 | 1.00 32.91 | CPS2 |
| ATOM | 1607 | 0 | GLY | 85 | 63.210 | 23.841 | 18.323 | 1.00 34.92 | CPS2 |
| MOTA | 1608 | N | LYS | 86 | 63.726 | 25.184 | 20.041 | 1.00 31.20 | CPS2 |
| ATOM | 1609 | CA | LYS | 86 | 63.781 | 26.379 | 19.203 | 1.00 29.67 | CPS2 |
| ATOM | 1610 | CB | LYS | 86 | 63.454 | 27.605 | 20.052 | 1.00 31.80 | CPS2 |
| ATOM | 1611 | CG | LYS | 86 | 62.137 | 27.394 | 20.790 | 1.00 34.73 | CPS2 |
| MOTA | 1612 | CD | LYS | 86 | 61.614 | 28.628 | 21.486 | 1.00 39.19 | CPS2 |
| MOTA | 1613 | CE | LYS | 86 | 60.239 | 28.331 | 22.094 | 1.00 41.01 | CPS2 |
| MOTA | 1614 | NZ | LYS | 86 | 59.558 | 29.559 | 22.592 | 1.00 43.57 | CPS2 |
| | 1615 | C | LYS | | | 26.492 | 18.541 | 1.00 28.23 | |
| ATOM | | | | 86 | 65.144 | | | | CPS2 |
| ATOM | 1616 | 0 | LYS | 86 | 66.169 | 26.212 | 19.159 | 1.00 27.95 | CPS2 |
| ATOM | 1617 | N | PRO | 87 | 65.173 | 26.922 | 17.272 | 1.00 27.01 | CPS2 |
| MOTA | 1618 | CD | PRO | 87 | 64.035 | 27.381 | 16.447 | 1.00 26.75 | CPS2 |
| MOTA | 1619 | CA | PRO | 87 | 66.427 | 27.050 | 16.534 | 1.00 25.49 | CPS2 |
| ATOM | 1620 | CB | PRO | 87 | 65.951 | 27.164 | 15.085 | 1.00 25.44 | CPS2 |
| ATOM | 1621 | CG | PRO | 87 | 64.735 | 28.043 | 15.239 | 1.00 27.74 | CPS2 |
| ATOM | 1622 | C | PRO | 87 | 67.379 | 28.185 | 16.881 | 1.00 24.72 | CPS2 |
| MOTA | 1623 | 0 | PRO | 87 | 66.979 | 29.270 | 17.306 | 1.00 23.36 | CPS2 |
| ATOM | 1624 | N | TYR | 88 | 68.664 | 27.904 | 16.716 | 1.00 22.58 | CPS2 |
| MOTA | 1625 | CA | TYR | 88 | 69.685 | 28.924 | 16.879 | 1.00 22.24 | CPS2 |
| ATOM | 1626 | CB | TYR | 88 | 70.208 | 29.052 | 18.324 | 1.00 22.46 | CPS2 |
| ATOM | 1627 | CG | TYR | 88 | 70.200 | 27.860 | 18.913 | 1.00 21.40 | CPS2 |
| | | | | | | | 19.577 | 1.00 21.74 | CPS2 |
| ATOM | 1628 | | TYR | 88 | 70.213 | 26.859 | | | |
| ATOM | 1629 | | TYR | 88 | 70.881 | 25.796 | 20.194 | 1.00 21.69 | CPS2 |
| ATOM | 1630 | CD2 | | 88 | 72.317 | 27.769 | 18.871 | 1.00 21.96 | CPS2 |
| ATOM | 1631 | CE2 | | 88 | 72.989 | 26.708 | 19.480 | 1.00 20.78 | CPS2 |
| ATOM | 1632 | CZ | TYR | 88 | 72.262 | 25.731 | 20.141 | 1.00 21.27 | CPS2 |
| ATOM | 1633 | OH | TYR | 88 | 72.923 | 24.699 | 20.772 | 1.00 20.50 | CPS2 |
| MOTA | 1634 | C | TYR | 88 | 70.781 | 28.522 | 15.912 | 1.00 22.02 | CPS2 |
| ATOM | 1635 | 0 | TYR | 88 | 70.897 | 27.352 | 15.550 | 1.00 23.05 | CPS2 |
| MOTA | 1636 | N | ILE | 89 | 71.577 | 29.485 | 15.480 | 1.00 21.04 | CPS2 |
| ATOM | 1637 | CA | ILE | 89 | 72.623 | 29.198 | 14.524 | 1.00 21.06 | CPS2 |
| MOTA | 1638 | CB | ILE | 89 | 72.573 | 30.209 | 13.369 | 1.00 21.84 | CPS2 |
| MOTA | 1639 | | ILE | 89 | 73.842 | 30.099 | 12.513 | 1.00 22.28 | CPS2 |
| MOTA | 1640 | | ILE | 89 | 71.324 | 29.982 | | 1.00 22.51 | CPS2 |
| | | | ILE | 89 | 71.172 | 31.035 | 11.407 | 1.00 23.39 | CPS2 |
| MOTA | 1641 | | | | | | | 1.00 23.35 | CPS2 |
| ATOM | 1642 | C | ILE | 89 | 74.043 | 29.228 | 15.072 | | |
| ATOM | 1643 | 0 | ILE | 89 | 74.401 | 30.123 | | 1.00 21.51 | CPS2 |
| # MOTA | 1644 | N | ILE | 90 | 74.839 | 28.248 | | 1.00 21.66 | CPS2 |
| MOTA | 1645 | CA | ILE | 90 | 76.255 | 28.184 | | 1.00 21.61 | CPS2 |
| MOTA | 1646 | CB | ILE | 90 | 76.641 | 26.878 | 15.727 | | CPS2 |
| ATOM | 1647 | CG2 | ILE | 90 | 78.169 | 26.743 | 15.791 | 1.00 22.23 | CPS2 |
| MOTA | 1648 | CG1 | ILE | 90 | 76.032 | 26.875 | 17.134 | 1.00 20.39 | CPS2 |
| MOTA | 1649 | | ILE | 90 | 76.542 | 27.991 | 18.041 | 1.00 20.47 | CPS2 |
| ATOM | 1650 | C | ILE | 90 | 77.019 | 28.232 | | 1.00 22.97 | CPS2 |
| ATOM | 1651 | ō | ILE | 90 | 76.763 | 27.437 | | 1.00 22.67 | CPS2 |
| ATOM | 1652 | И | CYS | 91 | 77.922 | 29.195 | | | CPS2 |
| WION | 1004 | 14 | CIJ | J 1 | 11.564 | 20020 | 20.000 | 2.00 20.00 | |

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|-------|------|------------|--------|----------|--------|--------|---------|------------|------|
| MOTA | 1653 | CA | CYS | 91 | 78.769 | 29.344 | 12.384 | 1.00 26.82 | CPS2 |
| MOTA | 1654 | CB | CYS | 91 | 78.229 | 30.414 | 11.432 | 1.00 26.17 | CPS2 |
| MOTA | 1655 | SG | CYS | 91 | 79.260 | 30.612 | 9.945 | 1.00 27.83 | CPS2 |
| MOTA | 1656 | C | CYS | 91 | 80.139 | 29.760 | 12.912 | 1.00 29.07 | CPS2 |
| ATOM | 1657 | 0 | CYS | 91 | 80.392 | 30.933 | 13.149 | 1.00 29.81 | CPS2 |
| MOTA | 1658 | N | THR | 92 | 81.011 | 28.784 | 13.114 | 1.00 33.43 | CPS2 |
| ATOM | 1659 | CA | THR | 92 | 82.347 | 29.049 | 13.637 | 1.00 37.11 | CPS2 |
| | | CB | | | | | | | |
| MOTA | 1660 | | THR | 92 | 83.080 | 27.726 | 13.883 | 1.00 38.23 | CPS2 |
| MOTA | 1661 | OG1 | | 92 | 82.422 | 27.027 | 14.947 | 1.00 38.10 | CPS2 |
| ATOM | 1662 | CG2 | | 92 | 84.536 | 27.971 | 14.260 | 1.00 40.35 | CPS2 |
| ATOM | 1663 | С | THR | 92 | 83.172 | 29.947 | 12.719 | 1.00 39.54 | CPS2 |
| ATOM | 1664 | 0 | THR | 92 | 84.071 | 30.663 | 13.177 | 1.00 40.49 | CPS2 |
| ATOM | 1665 | N | LYS | 93 | 82.846 | 29.916 | 11.432 | 1.00 40.59 | CPS2 |
| ATOM | 1666 | CA | LYS | 93 | 83.536 | 30.712 | 10.428 | 1.00 44.01 | CPS2 |
| ATOM | 1667 | CB | LYS | 93 | 83.024 | 30.334 | 9.040 | 1.00 45.12 | CPS2 |
| MOTA | 1668 | CG | LYS | 93 | 83.944 | 30.689 | 7.889 | 1.00 47.31 | CPS2 |
| ATOM | 1669 | CD | LYS | 93 | 83.519 | 29.921 | 6.650 | 1.00 47.58 | CPS2 |
| ATOM | 1670 | CE | LYS | 93 | 84.638 | 29.817 | 5.630 | 1.00 48.24 | CPS2 |
| ATOM | 1671 | NZ | LYS | 93 | 84.290 | 28.834 | 4.556 | 1.00 48.73 | CPS2 |
| | | | | | | | | | |
| ATOM | 1672 | C | LYS | 93 | 83.269 | 32.183 | 10.690 | 1.00 44.95 | CPS2 |
| ATOM | 1673 | 0 | LYS | 93 | 83.901 | 33.063 | 10.112 | 1.00 46.05 | CPS2 |
| AT'OM | 1674 | N | LEU | 94 | 82.322 | 32.443 | 11.575 | 1.00 45.51 | CPS2 |
| ATOM | 1675 | CA | LEU | 94 | 81.964 | 33.803 | 11.910 | 1.00 46.37 | CPS2 |
| ATOM | 1676 | CB | LEU | 94 | 80.452 | 33.898 | 12.120 | 1.00 46.46 | CPS2 |
| ATOM | 1677 | CG | LEU | 94 | 79.830 | 35.271 | 12.344 | 1.00 46.35 | CPS2 |
| ATOM | 1678 | CD1 | LEU | 94 | 80.037 | 36.148 | 11.121 | 1.00 47.12 | CPS2 |
| ATOM | 1679 | CD2 | LEU | 94 | 78.352 | 35.094 | 12.615 | 1.00 46.47 | CPS2 |
| ATOM | 1680 | C | LEU | 94 | 82.685 | 34.233 | 13.172 | 1.00 47.39 | CPS2 |
| MOTA | 1681 | 0 | LEU | 94 | 82.690 | 33.511 | 14.173 | 1.00 47.30 | CPS2 |
| MOTA | 1682 | N | SER | 95 | 83.319 | 35.401 | 13.116 | 1.00 48.63 | CPS2 |
| ATOM | 1683 | CA | SER | 95 | 84.015 | 35.941 | 14.278 | 1.00 48.81 | CPS2 |
| | | | | 95 95 | | | | 1.00 49.86 | CPS2 |
| ATOM | 1684 | CB | SER | | 84.347 | 37.420 | 14.037 | | |
| MOTA | 1685 | OG | SER | 95 | 83.229 | 38.121 | 13.511 | 1.00 51.01 | CPS2 |
| ATOM | 1686 | C | SER | 95 | 83.038 | 35.771 | 15.448 | 1.00 48.31 | CPS2 |
| ATOM | 1687 | 0 | SER | 95 | 81.843 | 35.585 | 15.221 | 1.00 48.26 | CPS2 |
| ATOM | 1688 | N | PRO | 96 | 83.524 | 35.840 | 16.704 | 1.00 46.89 | CPS2 |
| ATOM | 1689 | CD | PRO | 96 | 84.845 | 36.379 | 17.068 | 1.00 46.79 | CPS2 |
| ATOM | 1690 | CA | PRO | 96 | 82.693 | 35.682 | 17.909 | 1.00 45.46 | CPS2 |
| ATOM | 1691 | CB | PRO | 96 | 83.678 | 35.966 | 19.040 | 1.00 45.87 | CPS2 |
| ATOM | 1692 | CG | PRO | 96 | 84.573 | 36.988 | 18.434 | 1.00 45.85 | CPS2 |
| ATOM | 1693 | C | PRO | 96 | 81.431 | 36.544 | 18.033 | 1.00 44.28 | CPS2 |
| ATOM | 1694 | 0 | PRO | 96 | 81.041 | 36.911 | 19.141 | 1.00 45.08 | CPS2 |
| MOTA | 1695 | N | ALA | 97 | 80.782 | 36.839 | 16.913 | 1.00 41.71 | CPS2 |
| MOTA | 1696 | CA | ALA | 97 | 79.577 | 37.671 | 16.900 | 1.00 38.60 | CPS2 |
| MOTA | 1697 | CB | ALA | 97 | 79.384 | 38.246 | 15.507 | 1.00 39.14 | CPS2 |
| | | | ALA | | 78.288 | 36.977 | 17.347 | 1.00 36.55 | CPS2 |
| MOTA | 1698 | C | | 97 | | | | | CPS2 |
| ATOM | 1699 | 0 | ALA | 97 | 78.208 | 35.752 | 17.405 | 1.00 36.57 | |
| ATOM | 1700 | N | ALA | 98 | 77.274 | 37.784 | 17.651 | 1.00 33.65 | CPS2 |
| ATOM | 1701 | CA | ALA | 98 | 75.973 | 37.270 | 18.065 | 1.00 30.93 | CPS2 |
| MOTA | 1702 | CB | ALA | 98 | 75.295 | 38.239 | 19.026 | 1.00 29.97 | CPS2 |
| ATOM | 1703 | C | ALA | 98 | 75.125 | 37.106 | 16.804 | 1.00 28.95 | CPS2 |
| ATOM | 1704 | 0 | ALA | 98 | 75.077 | 37.990 | 15.949 | 1.00 28.62 | CPS2 |
| ATOM | 1705 | N | VAL | 99 | 74.454 | 35.969 | 16.709 | 1.00 26.50 | CPS2 |
| ATOM | 1706 | CA | VAL | 99 | 73.616 | 35.659 | 15.566 | 1.00 23.47 | CPS2 |
| ATOM | 1707 | CB | VAL | 99 | 74.179 | 34.437 | 14.806 | 1.00 23.08 | CPS2 |
| ATOM | 1708 | | VAL | 99 | 73.323 | 34.125 | 13.590 | 1.00 23.46 | CPS2 |
| | 1708 | | VAL | 99 | 75.617 | 34.718 | 14.381 | 1.00 24.82 | CPS2 |
| MOTA | 1103 | LG2 | A SATT | 23 | 13.01/ | 34.140 | T-4.20T | 1.00 21.02 | 0.00 |

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| MOTA | 1710 | С | VAL | 99 | 72.209 | 35.335 | 16.054 | 1.00 22.87 | CPS2 |
|------|--------------|-----|-----|-----|--------|--------|--------|------------|-------|
| MOTA | 1711 | 0 | VAL | 99 | 72.034 | 34.549 | 16.980 | 1.00 23.69 | CPS2 |
| MOTA | 1712 | N | HIS | 100 | 71.208 | 35.941 | 15.430 | 1.00 21.88 | CPS2 |
| MOTA | 1713 | CA | HIS | 100 | 69.819 | 35.685 | 15.800 | 1.00 20.93 | CPS2 |
| ATOM | 1714 | CB | HIS | 100 | 69.152 | 36.987 | 16.248 | 1.00 22.65 | CPS2 |
| MOTA | | CG | HIS | | | | | | |
| | 1715 | | | 100 | 69.930 | 37.726 | 17.296 | 1.00 24.71 | CPS2 |
| MOTA | 1716 | CD2 | | 100 | 70.837 | 38.727 | 17.191 | 1.00 26.85 | CPS2 |
| ATOM | 171 7 | NDI | HIS | 100 | 69.841 | 37.430 | 18.639 | 1.00 26.27 | CPS2 |
| ATOM | 1718 | CE1 | HIS | 100 | 70.658 | 38.217 | 19.318 | 1.00 28.01 | CPS2 |
| ATOM | 1719 | NE2 | HIS | 100 | 71.276 | 39.012 | 18.462 | 1.00 25.52 | CPS2 |
| ATOM | 1720 | C | HIS | 100 | 69.124 | 35.150 | 14.553 | 1.00 19.66 | CPS2 |
| ATOM | 1721 | ō | HIS | 100 | 69.414 | 35.596 | | 1.00 19.28 | CPS2 |
| | | | | | | | 13.445 | | |
| ATOM | 1722 | N | VAL | 101 | 68.208 | 34.203 | 14.729 | 1.00 20.06 | CPS2 |
| ATOM | 1723 | CA | VAL | 101 | 67.500 | 33.628 | 13.586 | 1.00 18.60 | CPS2 |
| MOTA | 1724 | CB | VAL | 101 | 68.111 | 32.251 | 13.166 | 1.00 18.24 | CPS2 |
| MOTA | 1725 | CG1 | VAL | 101 | 67.973 | 31.236 | 14.313 | 1.00 19.48 | CPS2 |
| MOTA | 1726 | CG2 | VAL | 101 | 67.436 | 31.719 | 11.884 | 1.00 16.59 | CPS2 |
| MOTA | 1727 | C | VAL | 101 | 66.053 | 33.403 | 13.982 | 1.00 19.22 | CPS2 |
| MOTA | 1728 | 0 | LAV | 101 | 65.753 | 33.247 | 15.160 | 1.00 20.38 | CPS2 |
| ATOM | 1729 | N | SER | 102 | 65.155 | 33.451 | 13.001 | 1.00 18.44 | CPS2 |
| ATOM | 1730 | | SER | 102 | | | 13.241 | 1.00 18.74 | |
| | | CA | | | 63.748 | 33.140 | | | CPS2 |
| ATOM | 1731 | CB | SER | 102 | 62.900 | 34.393 | 13.455 | 1.00 18.54 | CPS2 |
| ATOM | 1732 | OG | SER | 102 | 61.588 | 33.984 | 13.804 | 1.00 18.22 | CPS2 |
| ATOM | 1733 | C | SER | 102 | 63.270 | 32.398 | 12.006 | 1.00 18.15 | CPS2 |
| ATOM | 1734 | 0 | SER | 102 | 63.568 | 32.801 | 10.883 | 1.00 18.21 | CPS2 |
| ATOM | 1735 | N | ILE | 103 | 62.552 | 31.300 | 12.207 | 1.00 18.86 | CPS2 |
| ATOM | 1736 | CA | ILE | 103 | 62.054 | 30.511 | 11.079 | 1.00 18.76 | CPS2 |
| ATOM | 1737 | CB | ILE | 103 | 62.653 | 29.079 | 11.109 | 1.00 19.67 | CPS2 |
| MOTA | 1738 | | ILE | 103 | 62.224 | 28.298 | 9.869 | 1.00 21.39 | CPS2 |
| MOTA | 1739 | CG1 | ILE | 103 | 64.184 | 29.155 | 11.156 | 1.00 19.93 | CPS2 |
| MOTA | | | ILE | 103 | | 27.789 | 11.269 | 1.00 21.07 | CPS2 |
| | 1740 | | | | 64.862 | | | | |
| ATOM | 1741 | C | ILE | 103 | 60.537 | 30.418 | 11.198 | 1.00 19.92 | CPS2 |
| ATOM | 1742 | 0 | ILE | 103 | 60.004 | 30.291 | 12.307 | 1.00 21.12 | CPS2 |
| ATOM | 1743 | N | THR | 104 | 59.840 | 30.486 | 10.066 | 1.00 19.86 | CPS2 |
| MOTA | 1744 | CA | THR | 104 | 58.388 | 30.396 | 10.077 | 1.00 19.62 | CPS2 |
| ATOM | 1745 | CB | THR | 104 | 57.743 | 31.799 | 9.944 | 1.00 21.91 | CPS2 |
| ATOM | 1746 | OG1 | THR | 104 | 56.323 | 31.708 | 10.159 | 1.00 22.12 | CPS2 |
| ATOM | 1747 | CG2 | | 104 | 58.018 | 32.390 | 8.573 | 1.00 20.48 | CPS2 |
| ATOM | 1748 | C | THR | 104 | 57.945 | 29.487 | 8.934 | 1.00 20.91 | CPS2 |
| ATOM | 1749 | Ô | THR | 104 | 58.722 | 29.210 | 8.016 | 1.00 18.89 | CPS2 |
| | | | | | | | 8.999 | 1.00 20.52 | CPS2 |
| ATOM | 1750 | N | HIS | 105 | 56.705 | 29.015 | | | |
| MOTA | 1751 | CA | HIS | 105 | 56.179 | 28.108 | 7.973 | 1.00 24.14 | CPS2 |
| MOTA | 1752 | CB | HIS | 105 | 56.224 | 26.647 | | 1.00 27.48 | CPS2 |
| MOTA | 1753 | CG | HIS | 105 | 57.594 | 26.134 | 8.811 | 1.00 32.26 | CPS2 |
| MOTA | 1754 | CD2 | HIS | 105 | 58.267 | 26.095 | 9.987 | 1.00 33.69 | CPS2 |
| ATOM | 1755 | ND1 | HIS | 105 | 58.428 | 25.559 | 7.874 | 1.00 34.33 | CPS2 |
| ATOM | 1756 | | HIS | 105 | 59.555 | 25.191 | 8.457 | 1.00 33.58 | CPS2 |
| ATOM | 1757 | | HIS | 105 | 59.484 | 25.504 | 9.738 | 1.00 34.93 | CPS2 |
| | | | | | | | 7.653 | 1.00 23.87 | CPS2 |
| ATOM | 1758 | C | HIS | 105 | 54.702 | 28.393 | | | CPS2 |
| ATOM | 1759 | 0 | HIS | 105 | 53.974 | 28.944 | 8.476 | 1.00 23.81 | |
| ATOM | 1760 | N | THR | 106 | 54.284 | 28.013 | 6.449 | 1.00 23.91 | CPS2 |
| ATOM | 1761 | CA | THR | 106 | 52.875 | 28.065 | 6.054 | 1.00 24.84 | CPS2 |
| ATOM | 1762 | CB | THR | 106 | 52.484 | 29.199 | 5.058 | 1.00 24.13 | CPS2 |
| ATOM | 1763 | OG1 | THR | 106 | 53.116 | 28.984 | 3.792 | 1.00 25.72 | CPS2 |
| ATOM | 1764 | | THR | 106 | 52.841 | 30.571 | 5.616 | 1.00 24.87 | CPS2 |
| ATOM | 1765 | C | THR | 106 | 52.737 | 26,722 | 5.339 | 1.00 26.22 | CPS2 |
| ATOM | 1766 | | THR | 106 | 53.716 | 25.971 | 5.224 | 1.00 25.93 | CPS2 |
| AIOM | T / 00 | 0 | THK | 100 | 33./10 | 23.3/1 | J.424 | 1.00 23.73 | C1 02 |

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|------|------|-----|-------|-----|--------|--------|--------|------------|------|
| MOTA | 1767 | N | LYS | 107 | 51.544 | 26.408 | 4.857 | 1.00 27.42 | CPS2 |
| MOTA | 1768 | CA | LYS | 107 | 51.355 | 25.135 | 4.177 | 1.00 29.72 | CPS2 |
| MOTA | 1769 | CB | LYS | 107 | 49.913 | 25.013 | 3.676 | 1.00 32.60 | CPS2 |
| MOTA | 1770 | CG | LYS | 107 | 49.554 | 23.612 | 3.186 | 1.00 36.45 | CPS2 |
| MOTA | 1771 | CD | LYS | 107 | 48.151 | 23.568 | 2.586 | | |
| | | | | | | | | 1.00 39.60 | CPS2 |
| MOTA | 1772 | CE | LYS | 107 | 48.079 | 24.346 | 1.277 | 1.00 42.78 | CPS2 |
| MOTA | 1773 | NZ | LYS | 107 | 46.750 | 24.224 | 0.594 | 1.00 44.82 | CPS2 |
| MOTA | 1774 | С | LYS | 107 | 52.319 | 24.941 | 3.003 | 1.00 28.95 | CPS2 |
| MOTA | 1775 | 0 | LYS | 107 | 52.889 | 23.863 | 2.833 | 1.00 29.55 | CPS2 |
| ATOM | 1776 | N | GLU | 108 | 52.524 | 25.993 | 2.216 | 1.00 27.06 | CPS2 |
| ATOM | 1777 | CA | GLU | 108 | 53.374 | 25.916 | 1.033 | 1.00 27.06 | CPS2 |
| | | | | | | | | | |
| ATOM | 1778 | CB | GLU | 108 | 52.639 | 26.548 | -0.155 | 1.00 29.33 | CPS2 |
| ATOM | 1779 | CG | GLU | 108 | 51.301 | 25.907 | -0.494 | 1.00 36.04 | CPS2 |
| MOTA | 1780 | CD | GLU | 108 | 51.394 | 24.407 | -0.723 | 1.00 39.96 | CPS2 |
| MOTA | 1781 | OE1 | GLU | 108 | 52.416 | 23.935 | -1.270 | 1.00 43.61 | CPS2 |
| ATOM | 1782 | OE2 | GLU | 108 | 50.430 | 23.694 | -0.370 | 1.00 43.92 | CPS2 |
| ATOM | 1783 | C | GLU | 108 | 54.771 | 26.532 | 1.092 | 1.00 25.54 | CPS2 |
| ATOM | 1784 | 0 | GLU | 108 | 55.581 | 26.311 | 0.180 | 1.00 25.56 | CPS2 |
| MOTA | 1785 | | TYR | | 55.055 | | 2.138 | 1.00 24.09 | CPS2 |
| | | N | | 109 | | 27.305 | | | |
| MOTA | 1786 | CA | TYR | 109 | 56.350 | 27.982 | 2.250 | 1.00 21.97 | CPS2 |
| MOTA | 1787 | CB | TYR | 109 | 56.175 | 29.480 | 2.012 | 1.00 23.30 | CPS2 |
| MOTA | 1788 | CG | TYR | 109 | 55.611 | 29.823 | 0.664 | 1.00 24.68 | CPS2 |
| MOTA | 1789 | CD1 | TYR | 109 | 56.427 | 29.842 | -0.467 | 1.00 24.47 | CPS2 |
| ATOM | 1790 | CE1 | TYR | 109 | 55.895 | 30.083 | -1.731 | 1.00 25.63 | CPS2 |
| ATOM | 1791 | CD2 | | 109 | 54.248 | 30.062 | 0.505 | 1.00 25.42 | CPS2 |
| ATOM | 1792 | CE2 | TYR | 109 | 53.704 | 30.303 | -0.761 | 1.00 26.80 | CPS2 |
| | | | | | 54.530 | | | | CPS2 |
| ATOM | 1793 | CZ | TYR | 109 | | 30.307 | -1.866 | 1.00 25.17 | |
| ATOM | 1794 | OH | TYR | 109 | 53.996 | 30.501 | -3.118 | 1.00 28.15 | CPS2 |
| ATOM | 1795 | C | TYR | 109 | 57.069 | 27.849 | 3.578 | 1.00 21.24 | CPS2 |
| ATOM | 1796 | 0 | TYR | 109 | 56.465 | 27.578 | 4.616 | 1.00 20.80 | CPS2 |
| ATOM | 1797 | N | ALA | 110 | 58.379 | 28.067 | 3.518 | 1.00 21.00 | CPS2 |
| MOTA | 1798 | CA | ALA | 110 | 59.230 | 28.102 | 4.705 | 1.00 21.72 | CPS2 |
| MOTA | 1799 | CB | ALA | 110 | 60.238 | 26.966 | 4.686 | 1.00 22.11 | CPS2 |
| ATOM | 1800 | C | ALA | 110 | 59.945 | 29.450 | 4.560 | 1.00 21.05 | CPS2 |
| | | 0 | | | 60.301 | 29.852 | 3.451 | 1.00 20.79 | CPS2 |
| ATOM | 1801 | | ALA | 110 | | | | | |
| MOTA | 1802 | N | ALA | 111 | 60.141 | 30.165 | 5.657 | 1.00 20.04 | CPS2 |
| ATOM | 1803 | CA | ALA | 111 | 60.822 | 31.446 | 5.557 | 1.00 18.91 | CPS2 |
| ATOM | 1804 | CB | ALA | 111 | 59.802 | 32.577 | 5.431 | 1.00 18.42 | CPS2 |
| ATOM | 1805 | C | ALA | 111 | 61.683 | 31.648 | 6.785 | 1.00 17.86 | CPS2 |
| ATOM | 1806 | 0 | ALA | 111 | 61.400 | 31.111 | 7.847 | 1.00 17.82 | CPS2 |
| ATOM | 1807 | N | ALA | 112 | 62.754 | 32.411 | 6.638 | 1.00 18.38 | CPS2 |
| ATOM | 1808 | CA | ALA | 112 | 63.627 | 32.642 | 7,777 | 1.00 17.98 | CPS2 |
| ATOM | 1809 | CB | ALA | 112 | 64.718 | 31.564 | 7.820 | | CPS2 |
| | | | | | | | | 1.00 18.20 | CPS2 |
| ATOM | 1810 | C | ALA | 112 | 64.278 | 33.992 | 7.650 | | |
| MOTA | 1811 | 0 | ALA | 112 | 64.414 | 34.527 | 6.543 | 1.00 17.80 | CPS2 |
| MOTA | 1812 | N | GLN | 113 | 64.686 | 34.540 | 8.787 | 1.00 16.99 | CPS2 |
| MOTA | 1813 | CA | GLN | 113 | 65.406 | 35.802 | 8.775 | 1.00 19.02 | CPS2 |
| MOTA | 1814 | CB | GLN | 113 | 64.511 | 36.964 | 9.178 | 1.00 21.92 | CPS2 |
| ATOM | 1815 | CG | GLN | 113 | 64.045 | 36.908 | 10.593 | 1.00 24.71 | CPS2 |
| ATOM | 1816 | CD | GLN | 113 | 63.223 | 38.120 | 10.979 | | CPS2 |
| | | | | | | | | 1.00 29.66 | CPS2 |
| ATOM | 1817 | | GLN | 113 | 62.785 | 38.239 | | | CPS2 |
| ATOM | 1818 | | GLN | 113 | 63.001 | 39.019 | 10.028 | 1.00 31.94 | |
| MOTA | 1819 | C | GLN | 113 | 66.554 | 35.662 | 9.764 | 1.00 18.49 | CPS2 |
| ATOM | 1820 | 0 | GLN | 113 | 66.463 | 34.908 | 10.738 | 1.00 18.27 | CPS2 |
| ATOM | 1821 | N | VAL | 114 | 67.626 | 36.395 | 9.506 | 1.00 18.07 | CPS2 |
| ATOM | 1822 | CA | VAL | 114 | 68.811 | 36.355 | | 1.00 18.90 | CPS2 |
| ATOM | 1823 | СВ | VAL | 114 | 69.939 | 35.488 | 9.698 | 1.00 19.24 | CPS2 |
| AION | 1043 | بب | 4 277 | 444 | 02.555 | 33.400 | 2.030 | | |

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| ATOM | 1824 | CG1 | VAL | 114 | 71.288 | 35.715 | 10.406 | 1.00 20.55 | CPS2 |
|------|------|-----|-----|-----|----------------|--------|--------|------------|------|
| ATOM | 1825 | CG2 | VAL | 114 | 69.575 | 34.007 | 9.753 | 1.00 20.65 | CPS2 |
| MOTA | 1826 | C | VAL | 114 | 69.369 | 37.757 | 10.551 | 1.00 18.95 | CPS2 |
| MOTA | 1827 | 0 | VAL | 114 | 69.283 | 38.595 | 9.653 | 1.00 18.70 | CPS2 |
| MOTA | 1828 | N | VAL | 115 | 69.918 | 38.015 | 11.733 | 1.00 18.92 | CPS2 |
| MOTA | 1829 | CA | VAL | 115 | 70.580 | 39.291 | 11.989 | 1.00 19.34 | CPS2 |
| MOTA | 1830 | CB | VAL | 115 | 69.805 | 40.208 | 12.970 | 1.00 19.17 | CPS2 |
| MOTA | 1831 | CG1 | VAL | 115 | 70.668 | 41.445 | 13.298 | 1.00 20.91 | CPS2 |
| ATOM | 1832 | CG2 | VAL | 115 | 68.499 | 40.688 | 12.334 | 1.00 18.48 | CPS2 |
| ATOM | 1833 | C | VAL | 115 | 71.915 | 38.927 | 12.633 | 1.00 21.35 | CPS2 |
| ATOM | 1834 | 0 | VAL | 115 | 71.949 | 38.164 | 13.590 | 1.00 21.11 | CPS2 |
| ATOM | 1835 | N | ILE | 116 | 73.009 | 39.428 | 12.074 | 1.00 22.97 | CPS2 |
| ATOM | 1836 | CA | ILE | 116 | 74.333 | 39.174 | 12.641 | 1.00 25.35 | CPS2 |
| ATOM | 1837 | CB | ILE | 116 | 75.359 | 38.779 | 11.554 | 1.00 24.57 | CPS2 |
| ATOM | 1838 | CG2 | ILE | 116 | 76.752 | 38.641 | 12.177 | 1.00 25.34 | CPS2 |
| ATOM | 1839 | CG1 | ILE | 116 | 74.945 | 37.468 | 10.880 | 1.00 23.64 | CPS2 |
| ATOM | 1840 | CD1 | ILE | 116 | 75.862 | 37.065 | 9.734 | 1.00 24.45 | CPS2 |
| ATOM | 1841 | C | ILE | 116 | 74.763 | 40.511 | 13.243 | 1.00 27.82 | CPS2 |
| MOTA | 1842 | 0 | ILE | 116 | 74.692 | 41.531 | 12.569 | 1.00 26.14 | CPS2 |
| MOTA | 1843 | N | GLU | 117 | 75.176 | 40.508 | 14.508 | 1.00 31.83 | CPS2 |
| MOTA | 1844 | CA | GLU | 117 | 75.620 | 41.741 | 15.162 | 1.00 38.95 | CPS2 |
| MOTA | 1845 | CB | GLU | 117 | 75.075 | 41.848 | 16.583 | 1.00 40.48 | CPS2 |
| MOTA | 1846 | CG | GLU | 117 | 73.585 | 41.670 | 16.763 | 1.00 42.57 | CPS2 |
| ATOM | 1847 | CD | GLU | 117 | 73.180 | 41.900 | 18.211 | 1.00 43.48 | CPS2 |
| ATOM | 1848 | OEl | GLU | 117 | 73.040 | 43.075 | 18.613 | 1.00 45.02 | CPS2 |
| MOTA | 1849 | OE2 | GLU | 117 | 73.029 | 40.909 | 18.956 | 1.00 43.86 | CPS2 |
| MOTA | 1850 | C | GLU | 117 | 77.140 | 41.701 | 15.260 | 1.00 42.69 | CPS2 |
| ATOM | 1851 | 0 | GLU | 117 | 77.707 | 40.665 | 15.598 | 1.00 44.02 | CPS2 |
| ATOM | 1852 | N | ARG | 118 | 77.803 | 42.820 | 14.989 | 1.00 46.91 | CPS2 |
| ATOM | 1853 | CA | ARG | 118 | 79.259 | 42.843 | 15.069 | 1.00 50.26 | CPS2 |
| ATOM | 1854 | CB | ARG | 118 | 79.824 | 43.901 | 14.124 | 1.00 52.17 | CPS2 |
| MOTA | 1855 | CG | ARG | 118 | 79.547 | 45.337 | 14.529 | 1.00 54.69 | CPS2 |
| MOTA | 1856 | CD | ARG | 118 | 79 .478 | 46.208 | 13.288 | 1.00 57.22 | CPS2 |
| MOTA | 1857 | NE | ARG | 118 | 80.501 | 45.827 | 12.319 | 1.00 59.20 | CPS2 |
| MOTA | 1858 | CZ | ARG | 118 | 80.479 | 46.170 | 11.034 | 1.00 60.31 | CPS2 |
| MOTA | 1859 | NHI | ARG | 118 | 79.483 | 46.906 | 10.556 | 1.00 60.38 | CPS2 |
| ATOM | 1860 | NH2 | ARG | 118 | 81.451 | 45.769 | 10.224 | 1.00 60.45 | CPS2 |
| ATOM | 1861 | С | ARG | 118 | 79.722 | 43.108 | 16.499 | 1.00 51.12 | CPS2 |
| ATOM | 1862 | OTI | ARG | 118 | 78.849 | 43.285 | 17.380 | 1.00 51.54 | CPS2 |
| ATOM | 1863 | | ARG | 118 | 80.952 | 43.125 | 16.721 | 1.00 52.39 | CPS2 |
| ATOM | 1864 | C | GLY | 1 | 70.826 | 44.611 | 21.183 | 1.00 31.20 | CPS3 |
| MOTA | 1865 | 0 | GLY | 1 | 69.832 | 44.954 | 21.818 | 1.00 30.54 | CPS3 |
| MOTA | 1866 | N | GLY | 1 | 72.197 | 46.046 | 22.695 | 1.00 34.55 | CPS3 |
| MOTA | 1867 | CA | GLY | 1 | 72.168 | 45.285 | 21.411 | 1.00 32.26 | CPS3 |
| MOTA | 1868 | N | ILE | 2 | 70.797 | 43.643 | 20.274 | 1.00 29.14 | CPS3 |
| MOTA | 1869 | CA | ILE | 2 | 69.562 | 42.935 | 19.973 | 1.00 27.23 | CPS3 |
| MOTA | 1870 | CB | ILE | 2 | 69.544 | 42.452 | 18.510 | 1.00 28.42 | CPS3 |
| ATOM | 1871 | | ILE | 2 | 68.334 | 41.538 | 18.271 | 1.00 29.40 | CPS3 |
| MOTA | 1872 | | ILE | 2 | 69.495 | 43.670 | 17.576 | 1.00 28.86 | CPS3 |
| MOTA | 1873 | | ILE | 2 | 69.507 | 43.331 | 16.115 | 1.00 31.24 | CPS3 |
| ATOM | 1874 | C | ILE | 2 | 69.332 | 41.748 | 20.883 | 1.00 26.26 | CPS3 |
| ATOM | 1875 | 0 | ILE | 2 | 70.213 | 40.893 | 21.040 | 1.00 25.80 | CPS3 |
| MOTA | 1876 | N | TYR | 3 | 68.147 | 41.713 | 21.489 | 1.00 24.05 | CPS3 |
| MOTA | 1877 | CA | TYR | 3 | 67.752 | 40.622 | 22.369 | 1.00 24.41 | CPS3 |
| MOTA | 1878 | CB | TYR | 3 | 66.682 | 41.080 | 23.352 | 1.00 26.14 | CPS3 |
| ATOM | 1879 | CG | TYR | 3 | 66.254 | 39.967 | 24.268 | 1.00 28.89 | CPS3 |
| MOTA | 1880 | CD1 | TYR | 3 | 67.098 | 39.514 | 25.290 | 1.00 29.65 | CPS3 |
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| ATOM | 1881 | CE1 | TYR | 3 | 66.736 | 38.442 | 26.092 | 1.00 32.21 | CPS3 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| ATOM | 1882 | CD2 | TYR | 3 | 65.037 | 39.316 | 24.080 | 1.00 29.35 | CPS3 |
| ATOM | 1883 | | TYR | 3 | 64.667 | 38.235 | 24.883 | 1.00 31.35 | CPS3 |
| ATOM | 1884 | CZ | TYR | 3 | 65.520 | 37.806 | 25.881 | 1.00 32.89 | CPS3 |
| ATOM | 1885 | OH | TYR | 3 | 65.160 | 36.730 | 26.660 | 1.00 35.01 | CPS3 |
| ATOM | 1886 | C | TYR | 3 | 67.190 | 39.454 | 21.551 | 1.00 23.32 | CPS3 |
| ATOM | 1887 | ō | TYR | 3 | 67.604 | 38.305 | | | |
| ATOM | | | | | | | 21.720 | 1.00 22.34 | CPS3 |
| | 1888 | N | GLY | 4 | 66.240 | 39.755 | 20.667 | 1.00 21.28 | CPS3 |
| ATOM | 1889 | CA | GLY | 4 | 65.655 | 38.705 | 19.848 | 1.00 20.37 | CPS3 |
| ATOM | 1890 | C | GLY | 4 | 64.945 | 39.231 | 18.614 | 1.00 18.42 | CPS3 |
| ATOM | 1891 | 0 | GLY | 4 | 64.636 | 40.411 | 18.527 | 1.00 18.04 | CPS3 |
| ATOM | 1892 | N | ILE | 5 | 64.694 | 38.350 | 17.656 | 1.00 17.82 | CPS3 |
| ATOM | 1893 | CA | ILE | 5 | 63.990 | 38.736 | 16.432 | 1.00 17.02 | CPS3 |
| ATOM | 1894 | CB | ILE | 5 | 64.939 | 38.802 | 15.206 | 1.00 16.53 | CPS3 |
| MOTA | 1895 | CG2 | ILE | 5 | 66.110 | 39.753 | 15.514 | 1.00 17.11 | CPS3 |
| ATOM | 1896 | CG1 | ILE | 5 | 65.457 | 37.398 | 14.841 | 1.00 16.93 | CPS3 |
| MOTA | 1897 | CD1 | ILE | 5 | 66.404 | 37.390 | 13.622 | 1.00 18.91 | CPS3 |
| MOTA | 1898 | C | ILE | 5 | 62.932 | 37.669 | 16.202 | 1.00 17.16 | CPS3 |
| ATOM | 1899 | 0 | ILE | 5 | 63.033 | 36.555 | 16.737 | 1.00 16.49 | CPS3 |
| ATOM | 1900 | N | GLY | 6 | 61.900 | 38.010 | 15.441 | 1.00 16.65 | CPS3 |
| ATOM | 1901 | CA | GLY | 6 | 60.847 | 37.041 | 15.187 | 1.00 17.04 | CPS3 |
| ATOM | 1902 | C | GLY | 6 | 60.217 | 37.338 | 13.844 | 1.00 17.86 | CPS3 |
| ATOM | 1903 | ō | GLY | 6 | 60.070 | 38.500 | 13.472 | 1.00 16.46 | CPS3 |
| ATOM | 1904 | N | LEU | 7 | 59.865 | 36.283 | 13.110 | 1.00 18.17 | CPS3 |
| ATOM | 1905 | CA | LEU | 7 | 59.257 | 36.432 | 11.795 | 1.00 18.17 | CPS3 |
| | | | | 7 | | | | | |
| ATOM | 1906 | CB | LEU | | 60.258 | 36.047 | 10.698 | 1.00 17.40 | CPS3 |
| ATOM | 1907 | CG | LEU | 7 | 59.723 | 35.991 | 9.257 | 1.00 17.71 | CPS3 |
| MOTA | 1908 | | LEU | 7 | 59.370 | 37.420 | 8.785 | 1.00 18.00 | CPS3 |
| MOTA | 1909 | | LEU | 7 | 60.775 | 35.357 | 8.330 | 1.00 18.26 | CPS3 |
| MOTA | 1910 | C | LEU | 7 | 58.068 | 35.482 | 11.718 | 1.00 18.31 | CPS3 |
| MOTA | 1911 | 0 | LEU | 7 | 58.121 | 34.371 | 12.236 | 1.00 18.61 | CPS3 |
| ATOM | 1912 | N | ASP | 8 | 56.992 | 35.923 | 11.083 | 1.00 18.46 | CPS3 |
| MOTA | 1913 | CA | ASP | 8 | 55.849 | 35.043 | 10.911 | 1.00 18.86 | CPS3 |
| ATOM | 1914 | CB | ASP | 8 | 54.871 | 35.157 | 12.082 | 1.00 19.63 | CPS3 |
| MOTA | 1915 | CG | ASP | 8 | 53.642 | 34.294 | 11.881 | 1.00 22.43 | CPS3 |
| MOTA | 1916 | OD1 | ASP | 8 | 52.653 | 34.768 | 11.281 | 1.00 23.32 | CPS3 |
| MOTA | 1917 | OD2 | ASP | 8 | 53.683 | 33.126 | 12.294 | 1.00 24.61 | CPS3 |
| ATOM | 1918 | C | ASP | 8 | 55.107 | 35.350 | 9.632 | 1.00 19.01 | CPS3 |
| MOTA | 1919 | 0 | ASP | 8 | 54.955 | 36.507 | 9.251 | 1.00 19.92 | CPS3 |
| ATOM | 1920 | N | ILE | 9 | 54.671 | 34.302 | 8.946 | 1.00 18.64 | CPS3 |
| ATOM | 1921 | CA | ILE | 9 | 53.871 | 34.490 | 7.747 | 1.00 20.14 | CPS3 |
| MOTA | 1922 | CB | ILE | 9 | 54.565 | 33.982 | 6.468 | 1.00 19.98 | CPS3 |
| MOTA | 1923 | | ILE | 9 | 53.605 | 34.144 | 5.283 | 1.00 20.49 | CPS3 |
| ATOM | 1924 | | ILE | 9 | 55.843 | 34.782 | 6.213 | 1.00 20.86 | CPS3 |
| ATOM | 1925 | | ILE | 9 | 56.635 | 34.318 | 4.987 | 1.00 23.49 | CPS3 |
| ATOM | 1926 | C | ILE | 9 | 52.642 | 33.649 | 8.032 | 1.00 20.08 | CPS3 |
| ATOM | 1927 | 0 | ILE | 9 | 52.760 | 32.500 | 8.472 | 1.00 20.00 | CPS3 |
| | | | | | | | | 1.00 20.82 | CPS3 |
| ATOM | 1928 | N | THR | 10 | 51.470 | 34.224 | 7.793 | 1.00 20.82 | CPS3 |
| ATOM | 1929 | CA | THR | 10 | 50.218 | 33.543 | 8.064 | | |
| ATOM | 1930 | CB | THR | 10 | 49.502 | 34.213 | 9.267 | 1.00 23.80 | CPS3 |
| MOTA | 1931 | | THR | 10 | 50.237 | 33.942 | 10.478 | 1.00 22.74 | CPS3 |
| MOTA | 1932 | | THR | 10 | 48.088 | 33.667 | 9.413 | 1.00 24.86 | CPS3 |
| MOTA | 1933 | С | THR | 10 | 49.310 | 33.548 | 6.838 | 1.00 22.47 | CPS3 |
| MOTA | 1934 | 0 | THR | 10 | 49.106 | 34.581 | 6.197 | 1.00 22.06 | CPS3 |
| MOTA | 1935 | N | GLU | 11 | 48.784 | 32.377 | 6.508 | 1.00 23.62 | CPS3 |
| ATOM | 1936 | CA | GLU | 11 | 47.894 | 32.230 | 5.359 | 1.00 25.07 | CPS3 |
| MOTA | 1937 | CB | GLU | 11 | 47.846 | 30.757 | 4.940 | 1.00 25.66 | CPS3 |
| | | | | | | | | | |

| MOTA | 1938 | ÇG | GLU | 11 | 46.898 | 30.463 | 3.793 | 1.00 29.78 | CPS3 |
|------|------|-----|-----|----|--------|--------|--------|------------|-------|
| ATOM | 1939 | CD | GLU | 11 | 46.798 | 28.980 | 3.481 | 1.00 32.43 | CPS3 |
| ATOM | 1940 | OE1 | GLU | 11 | 47.101 | 28.151 | 4.373 | 1.00 34.21 | CPS3 |
| ATOM | 1941 | OE2 | GLU | 11 | 46.396 | 28.643 | 2.346 | 1.00 34.51 | CPS3 |
| MOTA | 1942 | C | GLU | 11 | 46.502 | 32.708 | 5.771 | 1.00 25.06 | CPS3 |
| MOTA | 1943 | 0 | GLU | 11 | 45.922 | 32.173 | 6.714 | 1.00 25.54 | CPS3 |
| MOTA | 1944 | N | LEU | 12 | 45.963 | 33.701 | 5.069 | 1.00 25.35 | CPS3 |
| MOTA | 1945 | CA | LEU | 12 | 44.642 | 34.234 | 5.403 | 1.00 26.43 | CPS3 |
| ATOM | 1946 | CB | LEU | 12 | 44.225 | 35.329 | 4.408 | 1.00 28.34 | CPS3 |
| MOTA | 1947 | CG | LEU | 12 | 44.432 | 36.787 | 4.846 | 1.00 30.12 | CPS3 |
| ATOM | 1948 | CD1 | LEU | 12 | 45.896 | 37.051 | 5.095 | 1.00 29.84 | CP\$3 |
| ATOM | 1949 | CD2 | LEU | 12 | 43.898 | 37.731 | 3.771 | 1.00 31.67 | CPS3 |
| ATOM | 1950 | С | LEU | 12 | 43.552 | 33.163 | 5.459 | 1.00 27.18 | CPS3 |
| MOTA | 1951 | 0 | LEU | 12 | 42.700 | 33.183 | 6.350 | 1.00 25.07 | CPS3 |
| MOTA | 1952 | N | ALA | 13 | 43.585 | 32.231 | 4.511 | 1.00 26.60 | CPS3 |
| MOTA | 1953 | CA | ALA | 13 | 42.602 | 31.160 | 4.467 | 1.00 27.39 | CPS3 |
| MOTA | 1954 | CB | ALA | 13 | 42.836 | 30.296 | 3.227 | 1.00 28.53 | CPS3 |
| MOTA | 1955 | C | ALA | 13 | 42.616 | 30.293 | 5.730 | 1.00 28.85 | CPS3 |
| ATOM | 1956 | 0 | ALA | 13 | 41.569 | 29.793 | 6.158 | 1.00 29.11 | CPS3 |
| ATOM | 1957 | N | ARG | 14 | 43.790 | 30.115 | 6.332 | 1.00 28.68 | CPS3 |
| ATOM | 1958 | CA | ARG | 14 | 43.898 | 29.303 | 7.536 | 1.00 29.64 | CPS3 |
| ATOM | 1959 | CB | ARG | 14 | 45.361 | 28.961 | 7.844 | 1.00 31.16 | CPS3 |
| ATOM | 1960 | CG | ARG | 14 | 45.520 | 27.811 | 8.831 | 1.00 33.62 | CPS3 |
| ATOM | 1961 | CD | ARG | 14 | 46.961 | 27.333 | 8.931 | 1.00 36.46 | CPS3 |
| ATOM | 1962 | NE | ARG | 14 | 47.813 | 28.263 | 9.669 | 1.00 39.10 | CPS3 |
| ATOM | 1963 | CZ | ARG | 14 | 47.809 | 28.400 | 10.993 | 1.00 39.42 | CPS3 |
| MOTA | 1964 | | ARG | 14 | 46.998 | 27.665 | 11.741 | 1.00 41.04 | CPS3 |
| MOTA | 1965 | | ARG | 14 | 48.618 | 29.273 | 11.572 | 1.00 39.96 | CPS3 |
| MOTA | 1966 | C | ARG | 14 | 43.277 | 30.067 | 8.693 | 1.00 30.10 | CPS3 |
| ATOM | 1967 | ō | ARG | 14 | 42.619 | 29.473 | 9.549 | 1.00 30.68 | CPS3 |
| ATOM | 1968 | N | ILE | 15 | 43.490 | 31.382 | 8.721 | 1.00 28.50 | CPS3 |
| ATOM | 1969 | CA | ILE | 15 | 42.904 | 32.220 | 9.765 | 1.00 29.44 | CPS3 |
| ATOM | 1970 | CB | ILE | 15 | 43.322 | 33.708 | 9.611 | 1.00 28.52 | CPS3 |
| ATOM | 1971 | CG2 | | 15 | 42.492 | 34.596 | 10.544 | 1.00 27.32 | CPS3 |
| ATOM | 1972 | | ILE | 15 | 44.809 | 33.865 | 9.955 | 1.00 27.87 | CPS3 |
| ATOM | 1973 | | ILE | 15 | 45.145 | 33.454 | 11.384 | 1.00 29.13 | CPS3 |
| ATOM | 1974 | C | ILE | 15 | 41.383 | 32.116 | 9.656 | 1.00 30.89 | CPS3 |
| ATOM | 1975 | 0 | ILE | 15 | 40.689 | 31.904 | 10.654 | 1.00 31.81 | CPS3 |
| ATOM | 1976 | N | ALA | 16 | 40.868 | 32.271 | 8.439 | 1.00 31.30 | CPS3 |
| MOTA | 1977 | CA | ALA | 16 | 39.427 | 32.180 | 8.223 | 1.00 33.08 | CPS3 |
| MOTA | 1978 | CB | ALA | 16 | 39.096 | 32.463 | 6.760 | 1.00 33.09 | CPS3 |
| MOTA | 1979 | С | ALA | 16 | 38.902 | 30.802 | 8.634 | 1.00 34.30 | CPS3 |
| MOTA | 1980 | 0 | ALA | 16 | 37.800 | 30.695 | 9.169 | 1.00 35.45 | CPS3 |
| ATOM | 1981 | N | SER | 17 | 39.689 | 29.753 | 8.395 | 1.00 35.66 | CPS3 |
| ATOM | 1982 | CA | SER | 17 | 39.282 | 28.396 | 8.764 | 1.00 38.32 | CPS3 |
| ATOM | 1983 | CB | SER | 17 | 40.271 | 27.356 | 8.227 | 1.00 39.07 | CPS3 |
| ATOM | 1984 | OG | SER | 17 | 40.290 | 27.332 | 6.810 | 1.00 40.78 | CPS3 |
| ATOM | 1985 | C | SER | 17 | 39.187 | 28.242 | 10.277 | 1.00 40.41 | CPS3 |
| ATOM | 1986 | 0 | SER | 17 | 38.202 | 27.704 | 10.789 | 1.00 40.87 | CPS3 |
| ATOM | 1987 | N | MET | 18 | 40.215 | 28.704 | 10.989 | 1.00 41.04 | CPS3 |
| MOTA | 1988 | CA | MET | 18 | 40.238 | 28.621 | 12.449 | 1.00 42.44 | CPS3 |
| MOTA | 1989 | CB | MET | 18 | 41.582 | 29.110 | 13.004 | 1.00 42.96 | CPS3 |
| MOTA | 1990 | CG | MET | 18 | 42.774 | 28.251 | 12.617 | 1.00 44.33 | CPS3 |
| MOTA | 1991 | SD | MET | 18 | 44.266 | 28.670 | 13.558 | 1.00 48.01 | CPS3 |
| ATOM | 1992 | CE | MET | 18 | 44.718 | 30.192 | 12.791 | 1.00 43.96 | CPS3 |
| ATOM | 1993 | C | MET | 18 | 39.115 | 29.448 | 13.055 | 1.00 42.50 | CPS3 |
| ATOM | 1994 | 0 | MET | 18 | 38.472 | 29.026 | 14.014 | 1.00 43.21 | CPS3 |
| ALON | エノノマ | ~ | | | 39.312 | 25.020 | 221 | | |

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| | | | | | | | | | | |
| | MOTA | 1995 | N | ALA | 19 | 38.886 | 30.629 | 12.496 | 1.00 43.10 | CPS3 |
| | ATOM | 1996 | CA | ALA | 19 | 37.838 | 31.517 | 12.981 | 1.00 44.50 | CPS3 |
| | ATOM | 1997 | CB | ALA | 19 | 37.901 | 32.844 | 12.233 | 1.00 45.06 | CPS3 |
| | MOTA | 1998 | C | ALA | 19 | 36.453 | 30.889 | 12.816 | 1.00 46.48 | CPS3 |
| | ATOM | 1999 | 0 | ALA | 19 | 35.541 | 31.155 | 13.603 | 1.00 46.54 | CPS3 |
| | ATOM | 2000 | N | GLY | 20 | 36.296 | 30.061 | 11.788 | 1.00 47.19 | CPS3 |
| | ATOM | 2001 | CA | GLY | 20 | 35.015 | 29.417 | 11.558 | 1.00 48.52 | CPS3 |
| | ATOM | 2002 2003 | C | GLY GLY | 20 20 | 34.838 33.754 | 28.190 27.928 | 12.429 12.945 | 1.00 48.97 1.00 49.64 | CPS3 |
| | ATOM ATOM | 2003 | O N | ARG | 21 | 35.734 | 27.328 | 12.545 | 1.00 49.84 | CPS3 CPS3 |
| | ATOM | 2004 | CA | ARG | 21 | 35.921 | 26.227 | 13.397 | 1.00 49.98 | CPS3 |
| | ATOM | 2005 | CB | ARG | 21 | 37.083 | 25.336 | 12.963 | 1.00 52.93 | CPS3 |
| | MOTA | 2007 | CG | ARG | 21 | 37.367 | 24.152 | 13.872 | 1.00 55.96 | CPS3 |
| | ATOM | 2008 | CD | ARG | 21 | 36.136 | 23.278 | 14.055 | 1.00 58.49 | CPS3 |
| | ATOM | 2009 | ΝE | ARG | 21 | 36.396 | 22.145 | 14.940 | 1.00 60.33 | CPS3 |
| | MOTA | 2010 | CZ | ARG | 21 | 35.448 | 21.371 | 15.457 | 1.00 60.98 | CPS3 |
| | MOTA | 2011 | NHl | ARG | 21 | 34.171 | 21.611 | 15.179 | 1.00 61.06 | CPS3 |
| | ATOM | 2012 | NH2 | ARG | 21 | 35.776 | 20.356 | 16.247 | 1.00 61.52 | CPS3 |
| at the la | MOTA | 2013 | C | ARG | 21 | 35.987 | 26.469 | 14.904 | 1.00 51.00 | CPS3 |
| all trades of the control of the con | MOTA | 2014 | 0 | ARG | 21 | 35.437 | 25.698 | 15.693 | 1.00 51.31 | CPS3 |
| and the contract of the contra | ATOM | 2015 | N | GLN | 22 | 36.655 | 27.543 | 15.307 | 1.00 50.09 | CPS3 |
| in | ATOM | 2016 | CA | GLN | 22 | 36.807 | 27.835 | 16.725 | 1.00 49.10 | CPS3 |
| 1 mg - 7: | ATOM | 2017 | CB | GLN | 22 | 38.224 | 28.330 | 17.011 | 1.00 48.88 | CPS3 CPS3 |
| en e | ATOM ATOM | 2018 2019 | CG CD | GLN GLN | 22 22 | 39.273 40.653 | 27.241 27.759 | 16.967 17.297 | 1.00 49.46 1.00 49.87 | CPS3 |
| | ATOM | 2019 | OE1 | | 22 | 40.828 | 28.529 | 18.242 | 1.00 50.04 | CPS3 |
| Charleston Charleston Charleston Charleston | ATOM | 2021 | NE2 | GLN | 22 | 41.648 | 27.330 | 16.526 | 1.00 50.52 | CPS3 |
| | ATOM | 2022 | C | GLN | 22 | 35.822 | 28.816 | 17.328 | 1.00 47.67 | CPS3 |
| | · ATOM | 2023 | 0 | GLN | 22 | 35.309 | 29.716 | 16.660 | 1.00 48.35 | CPS3 |
| A | MOTA | 2024 | N | LYS | 23 | 35.580 | 28.626 | 18.619 | 1.00 46.19 | CPS3 |
| en e | ATOM | 2025 | CA | LYS | 23 | 34.683 | 29.477 | 19.384 | 1.00 44.06 | CPS3 |
| The state of the s | ATOM | 2026 | CB | LYS | 23 | 34.086 | 28.701 | 20.569 | 1.00 45.41 | CPS3 |
| What program of the control of the | MOTA | 2027 | CG | LYS | 23 | 34.474 | 27.218 | 20.651 | 1.00 48.30 | CPS3 |
| | ATOM | 2028 | CD | LYS | 23 | 35.983 | 27.019 | 20.828 | 1.00 50.15 | CPS3 |
| Stranger laws | ATOM | 2029 | CE | LYS | 23 | 36.341 | 25.554 | 21.037 | 1.00 51.50 | CPS3 CPS3 |
| 1 | MOTA | 2030 | NZ | LYS LYS | 23 23 | 35.720 35.490 | 25.007 30.659 | 22.285 19.918 | 1.00 51.24 1.00 40.79 | CPS3 |
| | ATOM ATOM | 2031 2032 | C | LYS | 23 | 36.523 | 30.457 | 20.558 | 1.00 40.73 | CPS3 |
| | MOTA | 2032 | И | ARG | 24 | 35.029 | | 19.630 | 1.00 36.53 | CPS3 |
| | MOTA | 2033 | CA | ARG | 24 | 35.671 | 33.110 | 20.103 | 1.00 33.31 | CPS3 |
| | ATOM | 2035 | CB | ARG | 24 | 35,675 | 33.153 | 21.630 | 1.00 32.78 | CPS3 |
| | ATOM | 2036 | CG | ARG | 24 | 34.367 | 32.793 | 22.310 | 1.00 34.25 | CPS3 |
| | MOTA | 2037 | CD | ARG | 24 | 33.299 | 33.846 | 22.126 | 1.00 35.40 | CPS3 |
| | ATOM | 2038 | NE | ARG | 24 | 32.105 | 33.476 | 22.883 | 1.00 38.23 | CPS3 |
| | ATOM | 2039 | CZ | ARG | 24 | 30.866 | 33.783 | 22.520 | 1.00 38.00 | CPS3 |
| | MOTA | 2040 | | ARG | 24 | 30.653 | 34.474 | 21.405 | 1.00 38.06 | CPS3 |
| | MOTA | 2041 | | ARG | 24 | 29.841 | | 23.259 | 1.00 39.67 | CPS3 |
| 0 | MOTA | 2042 | С | ARG | 24 | 37.116 | 33.301 | 19.641 | 1.00 31.71 | CPS3 |
| | MOTA | 2043 | 0 | ARG | 24 | 37.930 | 33.845 | 20.393 | 1.00 27.62 1.00 29.27 | CPS3 CPS3 |
| | MOTA | 2044 | N | PHE | 25 | 37.441 | 32.880 | 18.421 | 1.00 29.27 | CPS3 |
| | ATOM | 2045 | CA | PHE | 25 25 | 38.816 | 33.016 32.446 | 17.950 16.539 | 1.00 28.40 | CPS3 |
| | MOTA | 2046 | CB CG | PHE PHE | 25 25 | 38.958 40.370 | 32.446 | 16.539 | 1.00 28.43 | CPS3 |
| | MOTA MOTA | 2047 2048 | | PHE. | 25 25 | 40.758 | 33.450 | 15.011 | 1.00 29.33 | CPS3 |
| | ATOM | 2049 | | PHE | 25 | 41.311 | 31.556 | 16.445 | 1.00 30.13 | CPS3 |
| | ATOM | 2050 | | PHE | 25 | 42.067 | | 14.618 | 1.00 30.52 | CPS3 |
| | ATOM | 2051 | | PHE | 25 | 42.625 | | 15.970 | 1.00 30.21 | CPS3 |
| | | | | | | | | | | |

| MOTA | 2052 | CZ | PHE | 25 | 42.997 | 32.570 | 15.059 | 1.00 29.47 | CPS3 |
|------|------|-----|-----|----|--------|--------|--------|---------------------|--------|
| MOTA | 2053 | C | PHE | 25 | 39.325 | 34.455 | 17.992 | 1.00 27.06 | CPS3 |
| MOTA | | 0 | PHE | 25 | | | | | |
| | 2054 | | | | 40.394 | 34.716 | 18.531 | 1.00 27.13 | CPS3 |
| MOTA | 2055 | N | ALA | 26 | 38.569 | 35.394 | 17.433 | 1.00 27.40 | CPS3 |
| MOTA | 2056 | CA | ALA | 26 | 38.996 | 36.793 | 17.441 | 1.00 26.90 | CPS3 |
| MOTA | 2057 | CB | ALA | 26 | 37.987 | 37.661 | 16.692 | 1.00 27.98 | CPS3 |
| ATOM | 2058 | C | ALA | 26 | 39.174 | 37.302 | 18.869 | 1.00 26.90 | CPS3 |
| MOTA | 2059 | 0 | ALA | 26 | 40.131 | 38.027 | 19.170 | 1.00 25.61 | CPS3 |
| MOTA | 2060 | N | GLU | 27 | 38.254 | 36.912 | 19.753 | 1.00 25.63 | CPS3 |
| MOTA | 2061 | CA | GLU | 27 | 38.314 | 37.329 | 21.143 | 1.00 25.29 | CPS3 |
| ATOM | 2062 | CB | GLU | 27 | 37.070 | 36.864 | 21.908 | 1.00 25.87 | CPS3 |
| ATOM | 2063 | CG | GLU | 27 | 35.815 | 37.656 | 21.612 | 1.00 26.46 | CPS3 |
| ATOM | 2064 | CD | GLU | 27 | 35.199 | 37.336 | 20.266 | 1.00 28.64 | CPS3 |
| ATOM | 2065 | | GLU | 27 | 35.569 | 36.324 | 19.633 | | CPS3 |
| | | | | | | | | 1.00 29.62 | |
| MOTA | 2066 | | GLU | 27 | 34.319 | 38.106 | 19.845 | 1.00 31.82 | CPS3 |
| ATOM | 2067 | С | GLU | 27 | 39.548 | 36.770 | 21.835 | 1.00 24.48 | CPS3 |
| ATOM | 2068 | 0 | GLU | 27 | 40.026 | 37.340 | 22.812 | 1.00 23.69 | CPS3 |
| MOTA | 2069 | N | ARG | 28 | 40.057 | 35.652 | 21.336 | 1.00 24.10 | CPS3 |
| MOTA | 2070 | CA | ARG | 28 | 41.235 | 35.046 | 21.937 | 1.00 25.35 | · CPS3 |
| MOTA | 2071 | CB | ARG | 28 | 41.286 | 33.561 | 21.588 | 1.00 26.74 | CPS3 |
| ATOM | 2072 | CG | ARG | 28 | 42.365 | 32.796 | 22.331 | 1.00 30.57 | CPS3 |
| MOTA | 2073 | CD | ARG | 28 | 42.064 | 31.303 | 22.339 | 1.00 33.01 | CPS3 |
| ATOM | 2074 | NE | ARG | 28 | 42.094 | 30.724 | 21.001 | 1.00 34.13 | CPS3 |
| ATOM | 2075 | CZ | ARG | 28 | 43.212 | 30.481 | 20.327 | 1.00 36.89 | CPS3 |
| ATOM | 2076 | | ARG | 28 | 44.389 | 30.768 | 20.871 | 1.00 37.04 | CPS3 |
| ATOM | 2077 | | ARG | 28 | 43.157 | 29.946 | 19.111 | 1.00 37.15 | CPS3 |
| ATOM | 2078 | C | ARG | 28 | 42.529 | 35.736 | 21.488 | 1.00 24.56 | CPS3 |
| | | | | 28 | | 35.730 | 22.282 | 1.00 24.30 | CPS3 |
| ATOM | 2079 | 0 | ARG | | 43.450 | | | | |
| ATOM | 2080 | N | ILE | 29 | 42.574 | 36.130 | 20.225 | 1.00 23.52 | CPS3 |
| ATOM | 2081 | CA | ILE | 29 | 43.760 | 36.773 | 19.657 | 1.00 24.20 | CPS3 |
| MOTA | 2082 | CB | ILE | 29 | 43.788 | 36.591 | 18.122 | 1.00 24.82 | CPS3 |
| MOTA | 2083 | | ILE | 29 | 45.074 | 37.184 | 17.538 | 1.00 25.66 | CPS3 |
| MOTA | 2084 | | ILE | 29 | 43.627 | 35.107 | 17.768 | 1.00 26.45 | CPS3 |
| MOTA | 2085 | CD1 | ILE | 29 | 44.675 | 34.207 | 18.357 | 1.00 26 <i>.</i> 17 | CPS3 |
| ATOM | 2086 | C | ILE | 29 | 43.866 | 38.270 | 19.932 | 1.00 24.20 | CPS3 |
| ATOM | 2087 | 0 | ILE | 29 | 44.964 | 38.795 | 20.164 | 1.00 23.59 | CPS3 |
| ATOM | 2088 | N | LEU | 30 | 42.722 | 38.952 | 19.913 | 1.00 22.23 | CPS3 |
| ATOM | 2089 | CA | LEU | 30 | 42.683 | 40.401 | 20.076 | 1.00 22.20 | CPS3 |
| ATOM | 2090 | СВ | LEU | 30 | 41.643 | 40.977 | 19.106 | 1.00 21.52 | CPS3 |
| ATOM | 2091 | CG | LEU | 30 | 41.738 | 40.518 | 17.649 | 1.00 22.01 | CPS3 |
| ATOM | 2092 | | LEU | 30 | 40.591 | 41.151 | 16.857 | 1.00 22.54 | CPS3 |
| ATOM | 2093 | | LEU | 30 | 43.104 | 40.926 | 17.051 | 1.00 22.99 | CPS3 |
| | 2093 | C | LEU | 30 | 42.387 | 40.940 | 21.467 | 1.00 22.82 | CPS3 |
| ATOM | | | | | | 40.342 | 22.216 | 1.00 22.70 | CPS3 |
| MOTA | 2095 | 0 | LEU | 30 | 41.622 | | | | CPS3 |
| MOTA | 2096 | N | THR | 31 | 42.995 | 42.080 | 21.798 | 1.00 22.58 | |
| MOTA | 2097 | CA | THR | 31 | 42.752 | 42.741 | 23.076 | 1.00 23.08 | CPS3 |
| MOTA | 2098 | CB | THR | 31 | 43.781 | 43.846 | 23.374 | 1.00 22.96 | CPS3 |
| ATOM | 2099 | OG1 | THR | 31 | 43.666 | 44.871 | 22.377 | 1.00 23.51 | CPS3 |
| ATOM | 2100 | CG2 | THR | 31 | 45.200 | 43.283 | 23.406 | 1.00 23.16 | CPS3 |
| ATOM | 2101 | С | THR | 31 | 41.400 | 43.438 | 22.944 | 1.00 23.05 | CPS3 |
| ATOM | 2102 | 0 | THR | 31 | 40.840 | 43.499 | 21.850 | 1.00 20.90 | CPS3 |
| ATOM | 2103 | N | ARG | 32 | 40.887 | 43.992 | 24.042 | 1.00 23.64 | CPS3 |
| ATOM | 2104 | CA | ARG | 32 | 39.593 | 44.672 | 23.984 | 1.00 25.29 | CPS3 |
| ATOM | 2105 | CB | ARG | 32 | 39.224 | 45.258 | 25.346 | 1.00 24.83 | CPS3 |
| ATOM | 2106 | CG | ARG | 32 | 39.005 | 44.220 | 26.419 | 1.00 26.80 | CPS3 |
| | | CD | ARG | 32 | 38.684 | 44.890 | 27.752 | 1.00 25.11 | CPS3 |
| ATOM | 2107 | | | | | | | 1.00 25.70 | CPS3 |
| ATOM | 2108 | ΝE | ARG | 32 | 38.513 | 43.908 | 28.819 | 1.00 23.70 | |

| T TO M | 2100 | 00 | BDQ | 2.2 | 20 261 | 44 030 | 20 201 | | |
|--------|------|-----|-----|-----|--------|--------|--------|------------|------|
| ATOM | 2109 | CZ | ARG | 32 | 38.361 | 44.218 | 30.101 | 1.00 25.97 | CPS3 |
| ATOM | 2110 | NHl | | 32 | 38.357 | 45.492 | 30.481 | 1.00 26.33 | CPS3 |
| MOTA | 2111 | NH2 | ARG | 32 | 38.224 | 43.256 | 31.005 | 1.00 27.07 | CPS3 |
| ATOM | 2112 | C | ARG | 32 | 39.570 | 45.789 | 22.953 | 1.00 25.39 | CPS3 |
| MOTA | 2113 | 0 | ARG | 32 | 38.608 | 45.912 | 22.187 | 1.00 24.58 | CPS3 |
| MOTA | 2114 | N | SER | 33 | 40.622 | 46.605 | 22.935 | 1.00 24.96 | CPS3 |
| MOTA | 2115 | CA | SER | 33 | 40.699 | 47.715 | 21.988 | 1.00 25.69 | CPS3 |
| MOTA | 2116 | CB | SER | 33 | 41.909 | 48.603 | 22.284 | 1.00 27.21 | CPS3 |
| ATOM | 2117 | OG | SER | 33 | 41.714 | 49.345 | 23.469 | 1.00 28.30 | CPS3 |
| ATOM | 2118 | C | SER | 33 | 40.766 | 47.250 | 20.544 | 1.00 25.41 | CPS3 |
| ATOM | 2119 | 0 | SER | 33 | 40.180 | | | | CPS3 |
| | | | | | | 47.870 | 19.664 | 1.00 25.68 | |
| ATOM | 2120 | N | GLU | 34 | 41.492 | 46.169 | 20.290 | 1.00 24.03 | CPS3 |
| ATOM | 2121 | CA | GLU | 34 | 41.597 | 45.640 | 18.935 | 1.00 23.95 | CPS3 |
| MOTA | 2122 | CB | GLU | 34 | 42.699 | 44.574 | 18.879 | 1.00 23.46 | CPS3 |
| MOTA | 2123 | CG | GLU | 34 | 44.089 | 45.163 | 19.059 | 1.00 21.69 | CPS3 |
| MOTA | 2124 | CD | GLU | 34 | 45.182 | 44.105 | 19.221 | 1.00 22.84 | CPS3 |
| MOTA | 2125 | OEl | GLU | 34 | 46.328 | 44.405 | 18.837 | 1.00 21.34 | CPS3 |
| MOTA | 2126 | OE2 | GLU | 34 | 44.900 | 42.996 | 19.740 | 1.00 20.06 | CPS3 |
| ATOM | 2127 | C | GLU | 34 | 40.244 | 45.051 | 18.516 | 1.00 25.26 | CPS3 |
| ATOM | 2128 | 0 | GLU | 34 | 39.846 | 45.151 | 17.353 | 1.00 25.38 | CPS3 |
| ATOM | 2129 | N | LEU | 35 | 39.548 | 44.433 | 19.472 | 1.00 24.79 | CPS3 |
| ATOM | 2130 | CA | LEU | 35 | 38.231 | 43.849 | 19.211 | 1.00 25.97 | CPS3 |
| ATOM | 2131 | CB | LEU | 35 | 37.678 | 43.160 | 20.462 | 1.00 27.07 | CPS3 |
| ATOM | 2132 | CG | LEU | 35 | 37.717 | 41.639 | 20.630 | 1.00 30.32 | CPS3 |
| ATOM | 2132 | | LEU | 35 | 36.834 | 41.312 | 21.844 | 1.00 30.54 | CPS3 |
| | | | | 35 | 37.201 | | 19.391 | 1.00 30.34 | CPS3 |
| ATOM | 2134 | | LEU | | | 40.893 | | | |
| ATOM | 2135 | C | LEU | 35 | 37.264 | 44.947 | 18.806 | 1.00 25.13 | CPS3 |
| MOTA | 2136 | 0 | LEU | 35 | 36.471 | 44.778 | 17.885 | 1.00 26.21 | CPS3 |
| MOTA | 2137 | N | ASP | 36 | 37.310 | 46.066 | 19.518 | 1.00 25.47 | CPS3 |
| MOTA | 2138 | CA | ASP | 36 | 36.432 | 47.180 | 19.189 | 1.00 26.39 | CPS3 |
| MOTA | 2139 | CB | ASP | 36 | 36.696 | 48.383 | 20.111 | 1.00 27.06 | CPS3 |
| ATOM | 2140 | CG | ASP | 36 | 36.203 | 48.148 | 21.531 | 1.00 30.18 | CPS3 |
| ATOM | 2141 | OD1 | ASP | 36 | 35.336 | 47.272 | 21.710 | 1.00 28.81 | CPS3 |
| ATOM | 2142 | OD2 | ASP | 36 | 36.667 | 48.843 | 22.464 | 1.00 29.67 | CPS3 |
| ATOM | 2143 | C | ASP | 36 | 36.638 | 47.580 | 17.733 | 1.00 28.21 | CPS3 |
| ATOM | 2144 | 0 | ASP | 36 | 35.674 | 47.866 | 17.024 | 1.00 27.00 | CPS3 |
| ATOM | 2145 | N | GLN | 37 | 37.892 | 47.580 | 17.281 | 1.00 28.66 | CPS3 |
| ATOM | 2146 | CA | GLN | 37 | 38.200 | 47.939 | 15.895 | 1.00 28.46 | CPS3 |
| ATOM | 2147 | CB | GLN | 37 | 39.712 | 48.129 | 15.705 | 1.00 31.40 | CPS3 |
| ATOM | 2148 | CG | GLN | 37 | 40.309 | 49.384 | 16.315 | 1.00 34.73 | CPS3 |
| MOTA | 2149 | CD | GLN | 37 | 41.820 | 49.462 | 16.104 | 1.00 37.78 | CPS3 |
| ATOM | 2150 | | GLN | 37 | 42.601 | 48.806 | 16.803 | 1.00 38.25 | CPS3 |
| ATOM | 2151 | NE2 | GLN | 37 | 42.233 | 50.256 | 15.128 | 1.00 40.09 | CPS3 |
| | | | | | | 46.838 | 14.954 | 1.00 28.42 | CPS3 |
| ATOM | 2152 | C | GLN | 37 | 37.729 | | | 1.00 28.42 | CPS3 |
| ATOM | 2153 | 0 | GLN | 37 | 37.107 | 47.097 | 13.918 | | |
| ATOM | 2154 | N | TYR | 38 | 38.040 | 45.602 | 15.322 | 1.00 25.92 | CPS3 |
| ATOM | 2155 | CA | TYR | 38 | 37.676 | 44.445 | 14.526 | 1.00 27.76 | CPS3 |
| ATOM | 2156 | CB | TYR | 38 | 38.124 | 43.179 | 15.268 | 1.00 26.65 | CPS3 |
| ATOM | 2157 | CG | TYR | 38 | 37.674 | 41.867 | 14.666 | 1.00 28.74 | CPS3 |
| ATOM | 2158 | CD1 | TYR | 38 | 36.522 | 41.225 | 15.130 | 1.00 27.49 | CPS3 |
| MOTA | 2159 | CE1 | TYR | 38 | 36.105 | 40.013 | 14.583 | 1.00 29.24 | CPS3 |
| MOTA | 2160 | CD2 | TYR | 38 | 38.397 | 41.264 | 13.636 | 1.00 27.76 | CPS3 |
| ATOM | 2161 | CE2 | | 38 | 37.986 | 40.046 | 13.081 | 1.00 29.24 | CPS3 |
| MOTA | 2162 | CZ | TYR | 38 | 36.840 | 39.430 | 13.565 | 1.00 29.43 | CPS3 |
| ATOM | 2163 | ОН | TYR | 38 | 36.440 | 38,218 | 13.057 | 1.00 30.36 | CPS3 |
| ATOM | 2164 | C | TYR | 38 | 36.177 | 44.398 | 14.219 | 1.00 28.73 | CPS3 |
| ATOM | 2165 | 0 | TYR | 38 | 35.776 | 44.169 | 13.075 | 1.00 28.54 | CPS3 |
| 7100 | 2103 | _ | 1 | 20 | 33.770 | 11,100 | | 2 | |
| | | | | | | | | | |

| ATOM | 2166 | N | TYR | 39 | 35.349 | 44.637 | 15.228 | 1.00 29.50 | CPS3 |
|------|------|---------|------------|----------|------------------|------------------|--------|------------|------|
| ATOM | 2167 | CA | TYR | 39 | 33.910 | 44.575 | 15.018 | 1.00 31.58 | CPS3 |
| ATOM | 2168 | CB | TYR | 39 | 33.195 | 44.515 | 16.367 | 1.00 31.24 | C2S3 |
| ATOM | 2169 | CG | TYR | 39 | 33.219 | 43.106 | 16.896 | 1.00 31.89 | CPS3 |
| ATOM | 2170 | CD1 | | 39 | 32.839 | 42.054 | 16.068 | 1.00 34.16 | CPS3 |
| ATOM | 2171 | CE1 | | 39 | 32.897 | 40.744 | 16.491 | 1.00 34.63 | CPS3 |
| ATOM | 2172 | CD2 | TYR | 39 | 33.658 | 42.808 | 18.185 | 1.00 34.03 | CPS3 |
| ATOM | 2173 | | TYR | 39 | 33.722 | 41.472 | 18.627 | 1.00 32.78 | |
| MOTA | 2174 | CZ | TYR | 39 | 33.722 | | | | CPS3 |
| ATOM | 2175 | | | | | 40.455 | 17.760 | 1.00 33.06 | CPS3 |
| | | OH | TYR | 39 | 33.404 | 39.126 | 18.112 | 1.00 36.81 | CPS3 |
| ATOM | 2176 | C | TYR | 39 | 33.277 | 45.627 | 14.110 | 1.00 33.88 | CPS3 |
| ATOM | 2177 | 0 | TYR | 39 | 32.122 | 45.484 | 13.715 | 1.00 34.54 | CPS3 |
| ATOM | 2178 | N | GLU | 40 | 34.026 | 46.666 | 13.766 | 1.00 35.41 | CPS3 |
| ATOM | 2179 | CA | GLU | 40 | 33.509 | 47.709 | 12.882 | 1.00 37.60 | CPS3 |
| ATOM | 2180 | CB | GLU | 40 | 34.045 | 49.077 | 13.302 | 1.00 39.04 | CPS3 |
| ATOM | 2181 | CG | GLU | 40 | 33.553 | 49.545 | 14.656 | 1.00 41.70 | CPS3 |
| MOTA | 2182 | CD | GLU | 40 | 32.040 | 49.515 | 14.755 | 1.00 44.23 | CPS3 |
| MOTA | 2183 | OE1 | | 40 | 31.374 | 50.110 | 13.879 | 1.00 46.21 | CPS3 |
| MOTA | 2184 | OE2 | GLU | 40 | 31.515 | 48.895 | 15.706 | 1.00 44.59 | CPS3 |
| MOTA | 2185 | С | GLU | 40 | 33.888 | 47.452 | 11.423 | 1.00 38.62 | CPS3 |
| ATOM | 2186 | 0 | GLU | 40 | 33.491 | 48.200 | 10.530 | 1.00 39.31 | CPS3 |
| MOTA | 2187 | N | LEU | 41 | 34.651 | 46.388 | 11.189 | 1.00 38.25 | CPS3 |
| MOTA | 2188 | CA | LEU | 41 | 35.120 | 46.028 | 9.851 | 1.00 37.52 | CPS3 |
| ATOM | 2189 | CB | LEU | 41 | 36.507 | 45.380 | 9.954 | 1.00 36.60 | CPS3 |
| ATOM | 2190 | CG | LEU | 41 | 37.764 | 46.251 | 10.003 | 1.00 37.26 | CPS3 |
| MOTA | 2191 | CD1 | LEU | 41 | 37.520 | 47.514 | 10.794 | 1.00 38.83 | CPS3 |
| ATOM | 2192 | CD2 | LEU | 41 | 38.906 | 45.436 | 10.604 | 1.00 35.48 | CPS3 |
| MOTA | 2193 | C | LEU | 41 | 34.206 | 45.080 | 9.079 | 1.00 37.57 | CPS3 |
| MOTA | 2194 | 0 | LEU | 41 | 33.441 | 44.317 | 9.662 | 1.00 36.05 | CPS3 |
| MOTA | 2195 | N | SER | 42 | 34.312 | 45.127 | 7.755 | 1.00 38.63 | CPS3 |
| MOTA | 2196 | CA | SER | 42 | 33.537 | 44.251 | 6.890 | 1.00 38.96 | CPS3 |
| MOTA | 2197 | CB | SER | 42 | 33.712 | 44.668 | 5.434 | 1.00 40.14 | CPS3 |
| ATOM | 2198 | OG | SER | 42 | 35.078 | 44.585 | 5.055 | 1.00 42.27 | CPS3 |
| ATOM | 2199 | C | SER | 42 | 34.102 | 42.849 | 7.077 | 1.00 39.70 | CPS3 |
| ATOM | 2200 | 0 | SER | 42 | 35.183 | 42.685 | 7.641 | 1.00 39.21 | CPS3 |
| ATOM | 2201 | N | ALA | 43 | 33.385 | 41.842 | 6.596 | 1.00 39.38 | CPS3 |
| MOTA | 2202 | CA | ALA | 43 | 33.844 | 40.463 | 6.721 | 1.00 40.19 | CPS3 |
| ATOM | 2203 | CB | ALA | 43 | 32.854 | 39.521 | 6.040 | 1.00 41.29 | CPS3 |
| ATOM | 2204 | C | ALA | 43 | 35.247 | 40.268 | 6.128 | 1.00 40.48 | CPS3 |
| ATOM | 2205 | 0 | ALA | 43 | 36.084 | 39.569 | 6.706 | 1.00 39.82 | CPS3 |
| ATOM | 2206 | N | LYS | 44 | 35.495 | 40.884 | 4.974 | 1.00 40.37 | CPS3 |
| ATOM | 2207 | CA | LYS | 44 | 36.786 | 40.767 | 4.305 | 1.00 40.57 | CPS3 |
| ATOM | 2208 | CB | LYS | 44 | 36.722 | 41.379 | 2.904 | 1.00 42.89 | CPS3 |
| ATOM | 2209 | CG | LYS | 44 | 38.039 | 41.314 | 2.139 | 1.00 45.09 | CPS3 |
| ATOM | 2210 | CD | LYS | 44 | 37.958 | 42.106 | 0.840 | 1.00 47.76 | CPS3 |
| ATOM | 2211 | CE | LYS | 44 | 39.309 | 42.177 | 0.145 | 1.00 49.05 | CPS3 |
| ATOM | 2212 | NZ | LYS | 44 | 39.300 | 43.158 | -0.980 | 1.00 50.90 | CPS3 |
| ATOM | 2212 | C | LYS | 44 | 37.886 | 41.454 | 5.097 | 1.00 39.09 | CPS3 |
| | 2213 | | LYS | 44 | 38.955 | 40.881 | 5.308 | 1.00 39.00 | CPS3 |
| ATOM | | 0 | | | | | 5.518 | 1.00 37.74 | CPS3 |
| ATOM | 2215 | N Ca | ARG ARG | 45 45 | 37.625 38.594 | 42.687 43.460 | 6.291 | 1.00 37.74 | CPS3 |
| ATOM | 2216 | CA | | | | | | 1.00 37.61 | CPS3 |
| ATOM | 2217 | CB | ARG | 45 | 38.073 | 44.882 | 6.517 | 1.00 37.81 | CPS3 |
| MOTA | 2218 | CG | ARG | 45 | 38.223 | 45.805 | 5.314 | 1.00 41.25 | CPS3 |
| MOTA | 2219 | CD | ARG | 45 | 39.693 | 46.134 | 5.076 | | CPS3 |
| MOTA | 2220 | NE | ARG | 45 | 40.264 | 46.872 | 6.203 | 1.00 45.35 | CPS3 |
| ATOM | 2221 | CZ | ARG | 45 | 41.392 | 46.536 | 6.826 | 1.00 46.41 | |
| ATOM | 2222 | NH1 | ARG | 45 | 42.078 | 45.469 | 6.435 | 1.00 46.39 | CPS3 |

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| MOTA | 2223 | NH2 | ARG | 45 | 41.833 | 47.269 | 7.843 | 1.00 46.62 | CPS3 |
|--------------|------|-----|-----|------------|--------|--------|--------|------------|------|
| ATOM | 2224 | С | ARG | 45 | 38.909 | 42.799 | 7.634 | 1.00 34.32 | CPS3 |
| ATOM | 2225 | 0 | ARG | 45 | 40.049 | 42.842 | 8.097 | 1.00 32.42 | CPS3 |
| ATOM | 2226 | N | LYS | 46 | 37.899 | 42.188 | 8.251 | 1.00 32.83 | CPS3 |
| ATOM | 2227 | CA | LYS | 46 | 38.075 | 41.509 | 9.532 | 1.00 31.12 | CPS3 |
| ATOM | 2228 | CB | LYS | 46 | 36.775 | 40.842 | 9.987 | 1.00 31.02 | CPS3 |
| ATOM | 2229 | CG | LYS | 46 | 35.746 | 41.775 | 10.599 | 1.00 30.98 | CPS3 |
| MOTA | 2230 | CD | LYS | 46 | 34.553 | 40.977 | 11.100 | 1.00 32.86 | CPS3 |
| MOTA | 2231 | CE | LYS | 46 | 33.524 | 41.861 | 11.785 | 1.00 34.98 | CPS3 |
| ATOM | 2232 | NZ | LYS | 46 | 32.360 | 41.053 | 12.230 | 1.00 37.21 | CPS3 |
| ATOM | 2233 | C | LYS | 46 | 39.148 | 40.438 | 9.434 | 1.00 30.57 | CPS3 |
| ATOM | 2234 | o | LYS | 46 | 40.025 | 40.352 | 10.293 | 1.00 28.78 | CPS3 |
| ATOM | 2235 | И | ASN | 47 | 39.061 | 39.612 | 8.392 | 1.00 29.54 | CPS3 |
| ATOM | 2236 | CA | ASN | 47 | 40.020 | 38.533 | 8.186 | 1.00 29.84 | CPS3 |
| ATOM | 2237 | CB | ASN | 47 | 39.589 | 37.671 | 6.989 | 1.00 31.31 | CPS3 |
| ATOM | 2238 | CG | ASN | 47 | 40.603 | 36.588 | 6.635 | 1.00 33.49 | CPS3 |
| ATOM | 2239 | | ASN | 47 | 40.838 | 35.651 | 7.400 | 1.00 34.63 | CPS3 |
| ATOM | 2240 | | ASN | 47 | 41.201 | 36.713 | 5.461 | 1.00 34.30 | CPS3 |
| ATOM | 2240 | C | ASN | 47 | 41.436 | 39.083 | 7.976 | 1.00 28.84 | CPS3 |
| ATOM | 2241 | 0 | ASN | 47 | 42.401 | 38.521 | 8.501 | 1.00 27.85 | CPS3 |
| ATOM | 2243 | N | GLU | 48 | 41.562 | 40.174 | 7.224 | 1.00 27.20 | CPS3 |
| ATOM | 2243 | CA | GLU | 48 | 42.881 | 40.779 | 6.988 | 1.00 27.86 | CPS3 |
| ATOM | 2245 | CB | GLU | 48 | 42.795 | 41.910 | 5.955 | 1.00 30.08 | CPS3 |
| ATOM | 2245 | CG | GLU | 48 | 42.755 | 41.492 | 4.580 | 1.00 34.36 | CPS3 |
| ATOM | 2247 | CD | GLU | 48 | 41.937 | 42.687 | 3.716 | 1.00 38.77 | CPS3 |
| ATOM | 2248 | | GLU | 48 | 41.356 | 42.477 | 2.627 | 1.00 40.99 | CPS3 |
| ATOM | 2249 | | GLU | 48 | 42.221 | 43.835 | 4.124 | 1.00 39.72 | CPS3 |
| ATOM | 2250 | C | GLU | 48 | 43.451 | 41.363 | 8.285 | 1.00 25.90 | CPS3 |
| MOTA | 2251 | 0 | GLU | 48 | 44.633 | 41.197 | 8.589 | 1.00 24.51 | CPS3 |
| MOTA | 2252 | N | PHE | 49 | 42.601 | 42.065 | 9.030 | 1.00 24.05 | CPS3 |
| | 2252 | CA | PHE | 49 | 42.995 | 42.688 | 10.293 | 1.00 24.45 | CPS3 |
| ATOM ATOM | 2254 | CB | PHE | 49 | 41.809 | 43.473 | 10.866 | 1.00 25.52 | CPS3 |
| ATOM | 2254 | CG | PHE | 49 | 42.073 | 44.119 | 12.203 | 1.00 26.02 | CPS3 |
| ATOM | 2256 | | PHE | 49 | 42.503 | 45.440 | 12.285 | 1.00 26.53 | CPS3 |
| ATOM | 2257 | | PHE | 49 | 41.842 | 43.419 | 13.385 | 1.00 26.09 | CPS3 |
| ATOM | 2258 | | PHE | 49 | 42.688 | 46.061 | 13.529 | 1.00 26.57 | CPS3 |
| MOTA | 2259 | | PHE | 49 | 42.028 | 44.027 | 14.630 | 1.00 25.34 | CPS3 |
| ATOM | 2260 | CZ | PHE | 49 | 42.448 | 45.350 | 14.702 | 1.00 24.86 | CPS3 |
| ATOM | 2261 | C | PHE | 49 | 43.431 | 41.603 | 11.278 | 1.00 24.05 | CPS3 |
| ATOM | 2262 | 0 | PHE | 49 | 44.499 | 41.691 | 11.885 | 1.00 22.16 | CPS3 |
| ATOM | 2263 | N | LEU | 50 | 42.597 | 40.577 | 11.429 | 1.00 23.09 | CPS3 |
| ATOM | 2264 | CA | LEU | 50 | 42.894 | 39.478 | 12.342 | 1.00 23.23 | CPS3 |
| MOTA | 2265 | CB | LEU | 50 | 41.727 | 38.488 | 12.348 | 1.00 24.42 | CPS3 |
| MOTA | 2266 | CG | LEU | 50 | 41.788 | 37.294 | 13.297 | 1.00 26.20 | CPS3 |
| ATOM | 2267 | | LEU | 50 | 42.039 | 37.735 | 14.751 | 1.00 26.62 | CPS3 |
| ATOM | 2268 | | LEU | 50 | 40.468 | 36.551 | 13.182 | 1.00 27.72 | CPS3 |
| ATOM | 2269 | C | LEU | 50 | 44.191 | 38.758 | 11.970 | 1.00 22.25 | CPS3 |
| ATOM | 2270 | ō | LEU | 50 | 45.033 | 38.483 | 12.835 | 1.00 21.88 | CPS3 |
| ATOM | 2271 | N | ALA | 51 | 44.359 | 38.455 | 10.685 | 1.00 21.04 | CPS3 |
| | 2272 | CA | ALA | 51 | 45.564 | 37.773 | 10.223 | 1.00 20.88 | CPS3 |
| ATOM ATOM | 2272 | CB | ALA | ,51 | 45.460 | 37.467 | 8.727 | 1.00 21.96 | CPS3 |
| ATOM | 2274 | C | ALA | ,51 51 | 46.815 | 38.615 | 10.497 | 1.00 21.09 | CPS3 |
| ATOM | 2274 | 0 | ALA | 51 | 47.860 | 38.077 | 10.863 | 1.00 20.76 | CPS3 |
| | 2276 | N | GLY | 52 | 46.698 | 39.929 | | 1.00 21.47 | CPS3 |
| ATOM | 2277 | CA | GLY | 52 | 47.830 | 40.814 | 10.559 | 1.00 20.85 | CPS3 |
| ATOM | 2278 | CA | GLY | 52 52 | 48.230 | 40.814 | | 1.00 21.87 | CPS3 |
| ATOM | 2278 | 0 | GLY | 52 52 | 48.230 | 40.871 | | | CPS3 |
| MOTA | 2219 | 9 | GLI | J 2 | 49.420 | 40.071 | 12.333 | | |

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| MOTA | 2280 | N | ARG | 53 | 47.234 | 40.907 | 12.908 | 1.00 20.71 | CPS3 |
|------|------|-----|-----|------------|--------|--------|---------|------------|------|
| MOTA | 2281 | CA | ARG | 53 | 47.489 | 40.953 | ,14.344 | 1.00 19.99 | CPS3 |
| MOTA | 2282 | CB | ARG | 53 | 46.188 | 41.249 | 15.102 | 1.00 21.12 | CPS3 |
| MOTA | 2283 | CG | ARG | 53 | 45.749 | 42.697 | 15.023 | 1.00 25.14 | CPS3 |
| MOTA | 2284 | CD | ARG | 53 | 46.854 | 43.589 | 15.542 | 1.00 26.59 | CPS3 |
| MOTA | 2285 | ΝE | ARG | 53 | 46.364 | 44.864 | 16.046 | 1.00 29.01 | CPS3 |
| ATOM | 2286 | CZ | ARG | 53 | 46.020 | 45.905 | 15.293 | 1.00 29.46 | CPS3 |
| MOTA | 2287 | NHl | ARG | 53 | 46.104 | 45.841 | 13.967 | 1.00 29.27 | CPS3 |
| MOTA | 2288 | NH2 | ARG | 53 | 45.615 | 47.028 | 15.882 | 1.00 26.91 | CPS3 |
| ATOM | 2289 | C | ARG | 53 | 48.067 | 39.628 | 14.802 | 1.00 18.67 | CPS3 |
| ATOM | 2290 | 0 | ARG | 53 | 48.983 | 39.585 | 15.623 | 1.00 19.03 | CPS3 |
| ATOM | 2291 | N | PHE | 54 | 47.524 | 38.541 | 14.274 | 1.00 19.10 | CPS3 |
| ATOM | 2292 | CA | PHE | 54 | 48.001 | 37.214 | 14.639 | 1.00 18.17 | CPS3 |
| ATOM | 2293 | CB | PHE | 54 | 47.145 | 36.157 | 13.926 | 1.00 20.62 | CPS3 |
| MOTA | 2294 | CG | PHE | 54 | 47.514 | 34.736 | 14.248 | 1.00 21.61 | CPS3 |
| ATOM | 2295 | CD1 | PHE | 54 | 48.429 | 34.050 | 13.462 | 1.00 22.92 | CPS3 |
| MOTA | 2296 | CD2 | PHE | 54 | 46.903 | 34.068 | 15.305 | 1.00 23.51 | CPS3 |
| MOTA | 2297 | CEl | PHE | 54 | 48.731 | 32.726 | 13.713 | 1.00 24.49 | CPS3 |
| MOTA | 2298 | CE2 | PHE | 54 | 47.196 | 32.735 | 15.572 | 1.00 24.31 | CPS3 |
| MOTA | 2299 | cz | PHE | 54 | 48.113 | 32.061 | 14.773 | 1.00 26.02 | CPS3 |
| MOTA | 2300 | С | PHE | 54 | 49.480 | 37.082 | 14.254 | 1.00 18.48 | CPS3 |
| ATOM | 2301 | 0 | PHE | 54 | 50.296 | 36.615 | 15.049 | 1.00 16.83 | CPS3 |
| ATOM | 2302 | N | ALA | 55 | 49.818 | 37.512 | 13.042 | 1.00 18.82 | CPS3 |
| ATOM | 2303 | CA | ALA | 55 | 51.202 | 37.426 | 12.564 | 1.00 19.23 | CPS3 |
| ATOM | 2304 | CB | ALA | 55 | 51.291 | 37.903 | 11.110 | 1.00 19.19 | CPS3 |
| ATOM | 2305 | C | ALA | 55 | 52.121 | 38.271 | 13.439 | 1.00 17.75 | CPS3 |
| MOTA | 2306 | 0 | ALA | 55 | 53.210 | 37.833 | 13.822 | 1.00 17.44 | CPS3 |
| ATOM | 2307 | N | ALA | 56 | 51.678 | 39.481 | 13.755 | 1.00 17.64 | CPS3 |
| ATOM | 2308 | CA | ALA | 56 | 52.490 | 40.382 | 14.572 | 1.00 17.27 | CPS3 |
| ATOM | 2309 | CB | ALA | 56 | 51.828 | 41.769 | 14.651 | 1.00 17.54 | CPS3 |
| MOTA | 2310 | C | ALA | 56 | 52.745 | 39.840 | 15.978 | 1.00 18.48 | CPS3 |
| MOTA | 2311 | 0 | ALA | 56 | 53.869 | 39.927 | 16.492 | 1.00 16.93 | CPS3 |
| MOTA | 2312 | N | LYS | 57 | 51.710 | 39.278 | 16.600 | 1.00 17.56 | CPS3 |
| MOTA | 2313 | CA | LYS | 57 | 51.864 | 38.758 | 17.953 | 1.00 17.39 | CPS3 |
| ATOM | 2314 | CB | LYS | 5 7 | 50.484 | 38.545 | 18.593 | 1.00 17.01 | CPS3 |
| ATOM | 2315 | CG | LYS | 5 7 | 49.741 | 39.852 | 18.728 | 1.00 17.00 | CPS3 |
| ATOM | 2316 | CD | LYS | 5 7 | 48.445 | 39.709 | 19.516 | 1.00 17.39 | CPS3 |
| ATOM | 2317 | CE | LYS | 5 7 | 47.650 | 41.015 | 19.466 | 1.00 17.65 | CPS3 |
| MOTA | 2318 | NZ | LYS | 57 | 46.589 | 41.049 | 20.526 | 1.00 18.42 | CPS3 |
| MOTA | 2319 | С | LYS | 5 7 | 52.694 | 37.492 | 17.958 | 1.00 18.30 | CPS3 |
| MOTA | 2320 | 0 | LYS | 57 | 53.456 | 37.248 | 18.895 | 1.00 17.97 | CPS3 |
| MOTA | 2321 | N | GLU | 58 | 52.555 | 36.692 | 16.903 | 1.00 19.29 | CPS3 |
| MOTA | 2322 | CA | GLU | 58 | 53.343 | 35.477 | 16.770 | 1.00 21.29 | CPS3 |
| MOTA | 2323 | CB | GLU | 58 | 52.885 | 34.710 | 15.518 | 1.00 25.54 | CPS3 |
| MOTA | 2324 | CG | GLU | 58 | 52.985 | 33.214 | 15.639 | 1.00 35.02 | CPS3 |
| MOTA | 2325 | CD | GLU | 58 | 52.321 | 32.682 | 16.899 | 1.00 36.12 | CPS3 |
| MOTA | 2326 | | GLU | 58 | 51.079 | 32.744 | 17.033 | 1.00 40.18 | CPS3 |
| MOTA | 2327 | | GLU | 58 | 53.059 | 32.207 | 17.772 | 1.00 38.83 | CPS3 |
| MOTA | 2328 | С | GLU | 58 | 54.818 | 35.900 | 16.644 | 1.00 20.21 | CPS3 |
| ATOM | 2329 | 0 | GLU | 58 | 55.696 | 35.365 | 17.335 | 1.00 19.40 | CPS3 |
| ATOM | 2330 | N | ALA | 59 | 55.089 | 36.867 | 15.768 | 1.00 16.40 | CPS3 |
| ATOM | 2331 | CA | ALA | 59 | 56.458 | 37.353 | 15.580 | | CPS3 |
| ATOM | 2332 | CB | ALA | 59 | 56.491 | 38.461 | 14.521 | 1.00 17.44 | CPS3 |
| MOTA | 2333 | C | ALA | 59 | 57.011 | 37.883 | 16.900 | 1.00 17.42 | CPS3 |
| ATOM | 2334 | 0 | ALA | 59 | 58.160 | 37.595 | 17.271 | | CPS3 |
| ATOM | 2335 | N | PHE | 60 | 56.200 | 38.657 | 17.613 | | CPS3 |
| ATOM | 2336 | CA | PHE | 60 | 56.655 | 39.219 | 18.882 | 1.00 17.55 | CPS3 |
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| MOTA | 2337 | CB | PHE | 60 | 55.586 | 40.128 | 19.502 | 1.00 17.91 | CPS3 |
|------|------|-----|-----|----------|--------|--------|--------|------------|------|
| ATOM | 2338 | CG | PHE | 60 | 55.984 | 40.684 | 20.847 | 1.00 18.76 | CPS3 |
| MOTA | 2339 | CD1 | PHE | 60 | 56.755 | 41.838 | 20.933 | 1.00 18.58 | CPS3 |
| ATOM | 2340 | CD2 | PHE | 60 | 55.659 | 40.001 | 22.021 | 1.00 19.49 | CPS3 |
| ATOM | 2341 | CE1 | | 60 | 57.212 | 42.309 | 22.172 | 1.00 20.20 | CPS3 |
| ATOM | 2342 | CE2 | | 60 | 56.107 | 40.459 | 23.266 | 1.00 20.93 | CPS3 |
| ATOM | 2343 | CZ | PHE | 60 | 56.886 | 41.612 | 23.341 | 1.00 20.99 | CPS3 |
| ATOM | 2344 | C | PHE | 60 | 57.008 | 38.118 | 19.883 | | |
| | | | | | | | | 1.00 18.91 | CPS3 |
| ATOM | 2345 | 0 | PHE | 60 | 58.053 | 38.173 | 20.543 | 1.00 18.95 | CPS3 |
| ATOM | 2346 | И | SER | 61 | 56.137 | 37.123 | 20.001 | 1.00 18.23 | CPS3 |
| MOTA | 2347 | CA | SER | 61 | 56.370 | 36.036 | 20.946 | 1.00 19.91 | CPS3 |
| MOTA | 2348 | CB | SER | 61 | 55.167 | 35.081 | 20.978 | 1.00 20.94 | CPS3 |
| ATOM | 2349 | OG | SER | 61 | 55.170 | 34.217 | 19.851 | 1.00 25.41 | CPS3 |
| MOTA | 2350 | С | SER | 61 | 57.642 | 35.256 | 20.618 | 1.00 21.39 | CPS3 |
| ATOM | 2351 | 0 | SER | 61 | 58.278 | 34.697 | 21.511 | 1.00 21.46 | CPS3 |
| MOTA | 2352 | N | LYS | 62 | 58.011 | 35.206 | 19.345 | 1.00 20.86 | CPS3 |
| ATOM | 2353 | CA | LYS | 62 | 59.227 | 34.500 | 18.958 | 1.00 23.14 | CPS3 |
| ATOM | 2354 | CB | LYS | 62 | 59.239 | 34.237 | 17.455 | 1.00 24.31 | CPS3 |
| MOTA | 2355 | CG | LYS | 62 | 58.295 | 33.143 | 17.003 | 1.00 28.06 | CPS3 |
| ATOM | 2356 | CD | LYS | 62 | 58.340 | 33.057 | 15.490 | 1.00 32.02 | CPS3 |
| ATOM | 2357 | CE | LYS | 62 | 58.060 | 31.655 | 14.987 | 1.00 34.92 | CPS3 |
| ATOM | 2358 | NZ | LYS | 62 | 58.159 | 31.623 | 13.510 | 1.00 35.49 | CPS3 |
| ATOM | 2359 | C | LYS | 62 | 60.444 | 35.343 | 19.340 | 1.00 22.30 | CPS3 |
| MOTA | 2360 | Ō | LYS | 62 | 61.464 | 34.815 | 19.788 | 1.00 23.20 | CPS3 |
| ATOM | 2361 | N | ALA | 63 | 60.337 | 36.654 | 19.156 | 1.00 19.62 | CPS3 |
| MOTA | 2362 | CA | ALA | 63 | 61.437 | 37.547 | 19.512 | 1.00 20.06 | CPS3 |
| ATOM | 2362 | CB | ALA | 63 | 61.145 | 38.960 | 19.019 | 1.00 20.10 | CPS3 |
| ATOM | | CB | ALA | 63 | 61.603 | 37.543 | 21.035 | 1.00 20.10 | CPS3 |
| | 2364 | | | | | | | | |
| ATOM | 2365 | 0 | ALA | 63 | 62.724 | 37.529 | 21.550 | 1.00 23.66 | CPS3 |
| ATOM | 2366 | N | PHE | 64 | 60.480 | 37.536 | 21.749 | 1.00 20.52 | CPS3 |
| ATOM | 2367 | CA | PHE | 64 | 60.502 | 37.548 | 23.209 | 1.00 23.24 | CPS3 |
| MOTA | 2368 | CB | PHE | 64 | 59.079 | 37.690 | 23.752 | 1.00 23.53 | CPS3 |
| MOTA | 2369 | CG | PHE | 64 | 59.023 | 38.051 | 25.211 | 1.00 24.99 | CPS3 |
| MOTA | 2370 | | PHE | 64 | 59.492 | 39.283 | 25.653 | 1.00 26.02 | CPS3 |
| ATOM | 2371 | | PHE | 64 | 58.488 | 37.163 | 26.135 | 1.00 25.12 | CPS3 |
| MOTA | 2372 | | PHE | 64 | 59.423 | 39.632 | 27.008 | 1.00 28.33 | CPS3 |
| MOTA | 2373 | CE2 | PHE | 64 | 58.412 | 37.495 | 27.484 | 1.00 26.52 | CPS3 |
| ATOM | 2374 | CZ | PHE | 64 | 58.877 | 38.729 | 27.924 | 1.00 27.24 | CPS3 |
| ATOM | 2375 | C | PHE | 64 | 61.140 | 36.251 | 23.718 | 1.00 25.44 | CPS3 |
| ATOM | 2376 | 0 | PHE | 64 | 61.688 | 36.204 | 24.826 | 1.00 24.64 | CPS3 |
| ATOM | 2377 | N | GLY | 65 | 61.039 | 35.202 | 22.910 | 1.00 26.62 | CPS3 |
| ATOM | 2378 | CA | GLY | 65 | 61.662 | 33.938 | 23.255 | 1.00 30.83 | CPS3 |
| ATOM | 2379 | С | GLY | 65 | 60.802 | 32.879 | 23.912 | 1.00 32.24 | CPS3 |
| ATOM | 2380 | 0 | GLY | 65 | 61.209 | 31.719 | 23.980 | 1.00 33.69 | CPS3 |
| MOTA | 2381 | N | THR | 66 | 59.616 | 33.256 | 24.376 | 1.00 32.78 | CPS3 |
| ATOM | 2382 | CA | THR | 66 | 58.733 | 32.302 | 25.043 | 1.00 34.27 | CPS3 |
| ATOM | 2383 | CB | THR | 66 | 57.991 | 32.969 | 26.200 | 1.00 35.66 | CPS3 |
| ATOM | 2384 | | THR | 66 | 57.122 | 33.978 | 25.668 | 1.00 37.64 | CPS3 |
| ATOM | 2385 | CG2 | | 66 | 58.969 | 33.610 | 27.179 | 1.00 34.33 | CPS3 |
| ATOM | 2386 | C | THR | 66 | 57.663 | 31.691 | 24.143 | 1.00 34.55 | CPS3 |
| ATOM | 2387 | 0 | THR | 66 | 57.154 | 30.610 | 24.431 | 1.00 34.19 | CPS3 |
| | 2388 | И | GLY | 67 | 57.320 | 32.376 | 23.054 | 1.00 34.33 | CPS3 |
| ATOM | | | | | | | 22.198 | 1.00 34.53 | CPS3 |
| MOTA | 2389 | CA | GLY | 67 67 | 56.256 | 31.877 | 22.136 | 1.00 34.85 | CPS3 |
| ATOM | 2390 | C | GLY | 67 67 | 54.962 | 32.175 | | 1.00 34.83 | CPS3 |
| ATOM | 2391 | 0 | GLY | 67 | 55.012 | 32.656 | 24.080 | | CPS3 |
| ATOM | 2392 | N | ILE | 68 | 53.808 | 31.915 | 22.338 | 1.00 35.31 | CPS3 |
| ATOM | 2393 | CA | ILE | 68 | 52.537 | 32.175 | 23.016 | 1.00 35.28 | CF33 |
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| MOTA | 2394 | CB | ILE | 68 | 51.389 | 32.407 | 22.011 | 1.00 34.11 | CPS3 |
|--------------|------|-----|-----|----------|--------|--------|--------|------------|------|
| MOTA | 2395 | CG2 | ILE | 68 | 50.052 | 32.474 | 22.755 | 1.00 32.62 | CPS3 |
| MOTA | 2396 | CG1 | ILE | 68 | 51.640 | 33.690 | 21.219 | 1.00 32.54 | CPS3 |
| MOTA | 2397 | CD1 | ILE | 68 | 51.647 | 34.958 | 22.063 | 1.00 32.72 | CPS3 |
| ATOM | 2398 | C | ILE | 68 | 52.161 | 30.999 | 23.910 | 1.00 36.56 | CPS3 |
| ATOM | 2399 | 0 | ILE | 68 | 52.085 | 29.862 | 23.447 | 1.00 36.53 | CPS3 |
| ATOM | 2400 | N | GLY | 69 | 51.922 | 31.279 | 25.187 | 1.00 36.84 | CPS3 |
| ATOM | 2401 | CA | GLY | 69 | 51.565 | 30.221 | 26.115 | 1.00 38.40 | CPS3 |
| ATOM | 2402 | C | GLY | 69 | 51.481 | 30.700 | 27.550 | 1.00 38.69 | CPS3 |
| ATOM | 2403 | 0 | GLY | 69 | 50.987 | 31.797 | 27.820 | 1.00 38.83 | CPS3 |
| MOTA | 2404 | N | ALA | 70 | 51.978 | 29.882 | 28.474 | 1.00 38.37 | CPS3 |
| MOTA | 2405 | CA | ALA | 70 | 51.949 | 30.215 | 29.895 | 1.00 37.89 | CPS3 |
| ATOM | 2406 | CB | ALA | 70 | 52.510 | 29.043 | 30.710 | 1.00 38.76 | CPS3 |
| ATOM | 2407 | C | ALA | 70 | 52.684 | 31.506 | 30.270 | 1.00 37.56 | CPS3 |
| ATOM | 2408 | 0 | ALA | 70 | 52.225 | 32.262 | 31.122 | 1.00 37.72 | CPS3 |
| MOTA | 2409 | N | GLN | 71 | 53.817 | 31.769 | 29.634 | 1.00 36.91 | CPS3 |
| MOTA | 2410 | CA | GLN | 71 | 54.590 | 32.965 | 29.954 | 1.00 36.41 | CPS3 |
| ATOM | 2411 | CB | GLN | 71 | 56.072 | 32.693 | 29.697 | 1.00 38.98 | CPS3 |
| MOTA | 2412 | CG | GLN | 71 | 56.540 | 31.358 | 30.251 | 1.00 42.83 | CPS3 |
| MOTA | 2413 | CD | GLN | 71 | 58.024 | 31.132 | 30.053 | 1.00 45.56 | CPS3 |
| ATOM | 2414 | | GLN | 71 | 58.854 | 31.783 | 30.695 | 1.00 47.59 | CPS3 |
| ATOM | 2415 | | GLN | 71 | 58.369 | 30.211 | 29.156 | 1.00 47.26 | CPS3 |
| ATOM | 2416 | C | GLN | 71 | 54.167 | 34.225 | 29.192 | 1.00 33.99 | CPS3 |
| MOTA | 2417 | ō | GLN | 71 | 54.514 | 35.332 | 29.585 | 1.00 34.52 | CPS3 |
| ATOM | 2418 | N | LEU | 72 | 53.422 | 34.056 | 28.107 | 1.00 30.98 | CPS3 |
| ATOM | 2419 | CA | LEU | 72 | 52.993 | 35.195 | 27.304 | 1.00 27.97 | CPS3 |
| ATOM | 2420 | CB | LEU | 72 | 54.108 | 35.592 | 26.333 | 1.00 26.71 | CPS3 |
| ATOM | 2421 | CG | LEU | 72 | 53.888 | 36.797 | 25.415 | 1.00 25.21 | CPS3 |
| MOTA | 2422 | | LEU | 72 | 54.008 | 38.103 | 26.212 | 1.00 25.07 | CPS3 |
| ATOM | 2423 | | LEU | 72 | 54.930 | 36.760 | 24.299 | 1.00 26.26 | CPS3 |
| ATOM | 2424 | C | LEU | 72 | 51.727 | 34.852 | 26.532 | 1.00 26.94 | CPS3 |
| MOTA | 2425 | 0 | LEU | 72 | 51.679 | 33.877 | 25.779 | 1.00 27.79 | CPS3 |
| ATOM | 2426 | N | SER | 73 | 50.706 | 35.673 | 26.723 | 1.00 24.63 | CPS3 |
| ATOM | 2427 | CA | SER | 73 | 49.416 | 35.486 | 26.081 | 1.00 24.89 | CPS3 |
| ATOM | 2428 | CB | SER | 73 | 48.318 | 35.677 | 27.135 | 1.00 26.50 | CPS3 |
| ATOM | 2429 | OG | SER | 73 | 47.068 | 35.913 | 26.531 | 1.00 28.99 | CPS3 |
| ATOM | 2430 | C | SER | 73 | 49.228 | 36.504 | 24.957 | 1.00 23.56 | CPS3 |
| ATOM | 2431 | ō | SER | 73 | 49.903 | 37.537 | 24.942 | 1.00 22.03 | CPS3 |
| ATOM | 2432 | N | PHE | 74 | 48.324 | 36.211 | 24.017 | 1.00 22.96 | CPS3 |
| ATOM | 2433 | CA | PHE | 74 | 48.016 | 37.150 | 22.933 | 1.00 21.51 | CPS3 |
| ATOM | 2434 | CB | PHE | 74 | 46.922 | 36.599 | 22.010 | 1.00 23.03 | CPS3 |
| MOTA | 2435 | CG | PHE | 74 | 47.386 | 35.535 | 21.060 | 1.00 24.56 | CPS3 |
| MOTA | 2436 | | PHE | 74 | 48.330 | 35.820 | 20.079 | 1.00 25.15 | CPS3 |
| MOTA | 2437 | | PHE | 74 | 46.854 | 34.246 | 21.127 | 1.00 26.66 | CPS3 |
| MOTA | 2438 | | PHE | 74 | 48.740 | 34.837 | 19.175 | 1.00 25.67 | CPS3 |
| MOTA | 2439 | | PHE | 74 | 47.257 | 33.251 | 20.226 | 1.00 27.19 | CPS3 |
| MOTA | 2440 | CZ | PHE | 74 | 48.200 | 33.547 | 19.251 | 1.00 26.99 | CPS3 |
| ATOM | 2441 | C | PHE | 74 | 47.476 | 38.424 | 23.573 | 1.00 22.00 | CPS3 |
| ATOM | 2441 | 0 | PHE | 74 | 47.624 | 39.519 | 23.038 | 1.00 20.92 | CPS3 |
| ATOM | 2442 | | GLN | 75 | 46.830 | 38.270 | 24.726 | 1.00 22.26 | CPS3 |
| ATOM | 2443 | CA | GLN | 75 75 | 46.830 | 39.402 | 25.431 | 1.00 22.23 | CPS3 |
| | 2444 | CB | GLN | 75 75 | 45.313 | 38.895 | 26.543 | 1.00 23.41 | CPS3 |
| ATOM | 2445 | CG | GLN | 75 75 | 44.119 | 38.109 | 26.025 | 1.00 25.20 | CPS3 |
| ATOM ATOM | 2446 | CD | GLN | 75 75 | 43.257 | 38.109 | 25.118 | 1.00 26.61 | CPS3 |
| ATOM | 2447 | | GLN | 75 75 | 43.257 | 40.080 | 25.118 | 1.00 27.48 | CPS3 |
| | | | GLN | 75 75 | 42.891 | 38.429 | 23.476 | 1.00 27.40 | CPS3 |
| ATOM | 2449 | | | | | 40.350 | 26.028 | 1.00 23.82 | CPS3 |
| MOTA | 2450 | С | GLN | 75 | 47.287 | 40.350 | 20.020 | 1.00 22.73 | 0100 |

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|------|------|-----|-----|----------|--------|--------|--------|------------|------|
| MOTA | 2451 | 0 | GLN | 75 | 46.962 | 41.486 | 26.389 | 1.00 21.60 | CPS3 |
| MOTA | 2452 | N | ASP | 76 | 48.532 | 39.890 | 26.146 | 1.00 21.97 | CPS3 |
| MOTA | 2453 | CA | ASP | 76 | 49.595 | 40.730 | 26.710 | 1.00 22.16 | CPS3 |
| MOTA | 2454 | CB | ASP | 76 | 50.738 | 39.876 | 27.279 | 1.00 22.82 | CPS3 |
| MOTA | 2455 | CG | ASP | 76 | 50.332 | 39.058 | 28.494 | 1.00 25.52 | CPS3 |
| ATOM | 2456 | OD1 | ASP | 76 | 49.557 | 39.565 | 29.332 | 1.00 25.20 | CPS3 |
| ATOM | 2457 | | ASP | 76 | 50.823 | 37.915 | 28.614 | 1.00 24.81 | CPS3 |
| ATOM | 2458 | C | ASP | 76 | 50.223 | 41.635 | 25.661 | 1.00 21.66 | CPS3 |
| | | | | | | | | | |
| ATOM | 2459 | 0 | ASP | 76 | 51.059 | 42.481 | 25.982 | 1.00 19.63 | CPS3 |
| ATOM | 2460 | N | ILE | 77 | 49.826 | 41.450 | 24.405 | 1.00 21.29 | CPS3 |
| MOTA | 2461 | CA | ILE | 77 | 50.416 | 42.202 | 23.301 | 1.00 19.67 | CPS3 |
| ATOM | 2462 | CB | ILE | 77 | 51.088 | 41.225 | 22.318 | 1.00 19.23 | CPS3 |
| ATOM | 2463 | CG2 | ILE | 77 | 51.893 | 41.995 | 21.253 | 1.00 18.53 | CPS3 |
| ATOM | 2464 | CG1 | ILE | 77 | 51.987 | 40.247 | 23.084 | 1.00 17.28 | CPS3 |
| ATOM | 2465 | CD1 | ILE | 77 | 52.313 | 38.989 | 22.257 | 1.00 19.10 | CPS3 |
| ATOM | 2466 | С | ILE | 77 | 49.379 | 42.988 | 22.520 | 1.00 20.27 | CPS3 |
| ATOM | 2467 | Ō | ILE | 77 | 48.401 | 42.416 | 22.062 | 1.00 20.00 | CPS3 |
| MOTA | 2468 | N | GLU | 78 | 49.603 | 44.288 | 22.354 | 1.00 21.09 | CPS3 |
| ATOM | 2469 | CA | GLU | 78 | 48.670 | 45.106 | 21.591 | 1.00 20.73 | CPS3 |
| | | | | 78 | 47.909 | 46.082 | 22.496 | 1.00 20.73 | CPS3 |
| ATOM | 2470 | CB | GLU | | | | | | |
| MOTA | 2471 | CG | GLU | 78 | 46.819 | 46.843 | 21.737 | 1.00 24.01 | CPS3 |
| ATOM | 2472 | CD | GLU | 78 | 45.862 | 47.584 | 22.651 | 1.00 27.03 | CPS3 |
| ATOM | 2473 | OE1 | | 78 | 46.036 | 48.806 | 22.844 | 1.00 28.55 | CPS3 |
| ATOM | 2474 | OE2 | GLU | 78 | 44.937 | 46.934 | 23.181 | 1.00 28.54 | CPS3 |
| ATOM | 2475 | C | GLU | 78 | 49.384 | 45.892 | 20.508 | 1.00 20.37 | CPS3 |
| ATOM | 2476 | 0 | GLU | 78 | 50.431 | 46.485 | 20.749 | 1.00 20.67 | CPS3 |
| ATOM | 2477 | N | ILE | 79 | 48.826 | 45.877 | 19.303 | 1.00 19.96 | CPS3 |
| MOTA | 2478 | CA | ILE | 79 | 49.420 | 46.642 | 18.212 | 1.00 19.14 | CPS3 |
| MOTA | 2479 | CB | ILE | 79 | 49.368 | 45.860 | 16.850 | 1.00 19.23 | CPS3 |
| MOTA | 2480 | CG2 | | 79 | 49.577 | 46.830 | 15.678 | 1.00 19.82 | CPS3 |
| MOTA | 2481 | CG1 | | 79 | 50.477 | 44.798 | 16.795 | 1.00 21.31 | CPS3 |
| ATOM | 2482 | CD1 | | 79 | 50.318 | 43.645 | 17.758 | 1.00 22.36 | CPS3 |
| ATOM | 2483 | C | ILE | 79 | 48.629 | 47.942 | 18.090 | 1.00 20.00 | CPS3 |
| | 2483 | o | ILE | 79 | 47.389 | 47.928 | 18.088 | 1.00 20.09 | CPS3 |
| ATOM | | | | | 49.340 | 49.068 | 18.028 | 1.00 19.20 | CPS3 |
| MOTA | 2485 | N | ARG | 80 | | | | | CPS3 |
| ATOM | 2486 | CA | ARG | 80 | 48.703 | 50.380 | 17.861 | 1.00 20.32 | |
| ATOM | 2487 | CB | ARG | 80 | 48.924 | 51.258 | 19.107 | 1.00 20.53 | CPS3 |
| ATOM | 2488 | CG | ARG | 80 | 48.340 | 50.644 | 20.380 | 1.00 21.77 | CPS3 |
| MOTA | 2489 | CD | ARG | 80 | 48.505 | 51.527 | 21.617 | 1.00 23.01 | CPS3 |
| ATOM | 2490 | NE | ARG | 80 | 47.957 | 50.833 | 22.780 | 1.00 23.15 | CPS3 |
| MOTA | 2491 | CZ | ARG | 80 | 48.032 | 51.267 | 24.038 | 1.00 25.30 | CPS3 |
| MOTA | 2492 | NH1 | ARG | 80 | 48.634 | 52.412 | 24.321 | 1.00 20.84 | CPS3 |
| MOTA | 2493 | NH2 | ARG | 80 | 47.511 | 50.536 | 25.014 | 1.00 26.37 | CPS3 |
| MOTA | 2494 | С | ARG | 80 | 49.349 | 51.037 | 16.640 | 1.00 20.88 | CPS3 |
| MOTA | 2495 | 0 | ARG | 80 | 50.362 | 50.550 | 16.138 | 1.00 20.01 | CPS3 |
| ATOM | 2496 | N | LYS | 81 | 48.755 | 52.123 | 16.148 | 1.00 21.43 | CPS3 |
| ATOM | 2497 | CA | LYS | 81 | 49.316 | 52.839 | | 1.00 22.45 | CPS3 |
| ATOM | 2498 | CB | LYS | 81 | 48.327 | 52.868 | | 1.00 25.71 | CPS3 |
| | | | | | | | 13.309 | | CPS3 |
| ATOM | 2499 | CG | LYS | 81 01 | 47.907 | 51.512 | | 1.00 34.29 | CPS3 |
| ATOM | 2500 | CD | LYS | 81 | 49.057 | 50.788 | | 1.00 34.23 | CPS3 |
| ATOM | 2501 | CE | LYS | 81 | 48.582 | 49.508 | | | |
| ATOM | 2502 | NZ | LYS | 81 | 47.631 | 49.799 | | 1.00 38.59 | CPS3 |
| ATOM | 2503 | C | LYS | 81 | 49.591 | 54.269 | 15.423 | 1.00 22.25 | CPS3 |
| ATOM | 2504 | 0 | LYS | 81 | 48.757 | 54.882 | 16.095 | 1.00 21.74 | CPS3 |
| ATOM | 2505 | N | ASP | 82 | 50.750 | 54.801 | | 1.00 21.32 | CPS3 |
| MOTA | 2506 | CA | ASP | 82 | 51.055 | 56.169 | 15.411 | | CPS3 |
| ATOM | 2507 | CB | ASP | 82 | 52.568 | 56.396 | 15.564 | 1.00 23.73 | CPS3 |
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| 7.00 | 2522 | 00 | 3.00 | 0.0 | E2 240 | EC 202 | 14 252 | 1 00 05 37 | 0703 |
|------|------|-----|----------------------|-----|--------|--------|--------|------------|------|
| ATOM | 2508 | | ASP | 82 | 53.340 | 56.303 | 14.253 | 1.00 25.37 | CPS3 |
| MOTA | 2509 | ODl | | 82 | 52.736 | 56.371 | 13.161 | 1.00 25.70 | CPS3 |
| MOTA | 2510 | OD2 | ASP | 82 | 54.585 | 56.182 | 14.331 | 1.00 27.40 | CPS3 |
| MOTA | 2511 | C | ASP | 82 | 50.446 | 57.129 | 14.394 | 1.00 26.03 | CPS3 |
| MOTA | 2512 | 0 | ASP | 82 | 49.682 | 56.711 | 13.518 | 1.00 25.08 | CPS3 |
| ATOM | 2513 | N | GLN | 83 | 50.783 | 58.406 | 14.521 | 1.00 27.30 | CPS3 |
| ATOM | 2514 | CA | GLN | 83 | 50.243 | 59.439 | 13.648 | 1.00 30.37 | CPS3 |
| ATOM | 2515 | CB | GLN | 83 | 50.694 | 60.810 | 14.158 | 1.00 32.92 | CPS3 |
| | 2516 | CG | GLN | 83 | 50.035 | 61.193 | 15.481 | 1.00 36.66 | CPS3 |
| ATOM | | | | | | | | | |
| ATOM | 2517 | CD | GLN | 83 | 48.633 | 61.738 | 15.292 | 1.00 40.09 | CPS3 |
| MOTA | 2518 | OE1 | | 83 | 48.448 | 62.940 | 15.079 | 1.00 42.06 | CPS3 |
| MOTA | 2519 | NE2 | GLN | 83 | 47.637 | 60.859 | 15.354 | 1.00 40.07 | CPS3 |
| ATOM | 2520 | C | GLN | 83 | 50.587 | 59.276 | 12.167 | 1.00 30.09 | CPS3 |
| ATOM | 2521 | 0 | GLN | 83 | 49.900 | 59.834 | 11.308 | 1.00 30.34 | CPS3 |
| ATOM | 2522 | N | ASN | 84 | 51.647 | 58.532 | 11.865 | 1.00 29.03 | CPS3 |
| ATOM | 2523 | CA | ASN | 84 | 52.024 | 58.296 | 10.471 | 1.00 29.59 | CPS3 |
| ATOM | 2524 | СВ | ASN | 84 | 53.544 | 58.202 | 10.303 | 1.00 31.65 | CPS3 |
| MOTA | 2525 | CG | ASN | 84 | 54.239 | 59.536 | 10.457 | 1.00 34.87 | CPS3 |
| ATOM | 2526 | OD1 | | 84 | 53.732 | 60.566 | 10.022 | 1.00 36.47 | CPS3 |
| | | | | | | 59.520 | 11.060 | 1.00 36.00 | CPS3 |
| ATOM | 2527 | ND2 | | 84 | 55.425 | | | | |
| MOTA | 2528 | C | ASN | 84 | 51.419 | 56.990 | 9.974 | 1.00 28.93 | CPS3 |
| ATOM | 2529 | 0 | ASN | 84 | 51.609 | 56.613 | 8.815 | 1.00 30.32 | CPS3 |
| MOTA | 2530 | N | GLY | 85 | 50.712 | 56.286 | 10.852 | 1.00 26.33 | CPS3 |
| MOTA | 2531 | CA | GLY | 85 | 50.116 | 55.019 | 10.464 | 1.00 24.71 | CPS3 |
| ATOM | 2532 | C | GLY | 85 | 51.063 | 53.851 | 10.697 | 1.00 23.82 | CPS3 |
| ATOM | 2533 | 0 | GLY | 85 | 50.759 | 52.713 | 10.341 | 1.00 24.11 | CPS3 |
| ATOM | 2534 | N | LYS | 86 | 52.214 | 54.131 | 11.302 | 1.00 21.10 | CPS3 |
| ATOM | 2535 | CA | LYS | 86 | 53.204 | 53.096 | 11.582 | 1.00 21.62 | CPS3 |
| ATOM | 2536 | CB | LYS | 86 | 54.561 | 53.738 | 11.883 | 1.00 21.42 | CPS3 |
| MOTA | 2537 | CG | LYS | 86 | 55.625 | 52.760 | 12.401 | 1.00 23.00 | CPS3 |
| | 2538 | CD | LYS | 86 | 56.097 | 51.789 | 11.325 | 1.00 22.60 | CPS3 |
| ATOM | | | | | | | 11.921 | 1.00 21.76 | CPS3 |
| ATOM | 2539 | CE | LYS | 86 | 57.073 | 50.766 | | 1.00 21.78 | CPS3 |
| MOTA | 2540 | NZ | LYS | 86 | 57.761 | 49.970 | 10.852 | | |
| MOTA | 2541 | С | LYS | 86 | 52.782 | 52.244 | 12.783 | 1.00 20.36 | CPS3 |
| ATOM | 2542 | 0 | LYS | 86 | 52.468 | 52.776 | 13.843 | 1.00 20.19 | CPS3 |
| MOTA | 2543 | N | PRO | 87 | 52.770 | 50.912 | 12.632 | 1.00 20.59 | CPS3 |
| ATOM | 2544 | CD | PRO | 87 | 52.925 | 50.084 | 11.423 | 1.00 21.13 | CPS3 |
| ATOM | 2545 | CA | PRO | 87 | 52.375 | 50.091 | 13.781 | 1.00 20.38 | CPS3 |
| ATOM | 2546 | CB | PRO | 87 | 52.082 | 48.729 | 13.160 | 1.00 22.01 | CPS3 |
| ATOM | 2547 | CG | PRO | 87 | 53.044 | 48.675 | 12.009 | 1.00 23.44 | CPS3 |
| ATOM | 2548 | C | PRO | 87 | 53.481 | 49.991 | 14.812 | 1.00 18.94 | CPS3 |
| ATOM | 2549 | ō | PRO | 87 | 54.662 | 49.996 | 14.468 | 1.00 18.59 | CPS3 |
| | 2550 | N | TYR | 88 | 53.092 | 49.938 | 16.082 | 1.00 18.68 | CPS3 |
| ATOM | | | | | 54.064 | 49.757 | 17.155 | 1.00 18.87 | CPS3 |
| MOTA | 2551 | CA | TYR | 88 | | | 17.734 | 1.00 19.03 | CPS3 |
| ATOM | 2552 | CB | TYR | 88 | 54.566 | 51.093 | | | CPS3 |
| MOTA | 2553 | CG | TYR | 88 | 53.531 | 51.940 | 18.426 | 1.00 19.37 | |
| MOTA | 2554 | CD1 | TYR | 88 | 53.395 | 51.915 | 19.804 | 1.00 19.95 | CPS3 |
| MOTA | 2555 | CE1 | TYR | 88 | 52.413 | 52.683 | 20.449 | 1.00 20.13 | CPS3 |
| MOTA | 2556 | CD2 | TYR | 88 | 52.665 | 52.756 | 17.693 | 1.00 19.40 | CPS3 |
| ATOM | 2557 | CE2 | TYR | 88 | 51.690 | 53.519 | 18.315 | 1.00 19.13 | CPS3 |
| ATOM | 2558 | CZ | TYR | 88 | 51.562 | 53.479 | 19.691 | 1.00 18.55 | CPS3 |
| ATOM | 2559 | OH | TYR | 88 | 50.568 | 54.204 | 20.299 | 1.00 19.71 | CPS3 |
| ATOM | 2560 | C | TYR | 88 | 53.385 | 48.899 | 18.211 | 1.00 18.42 | CPS3 |
| | | | TYR | 88 | 52.159 | 48.825 | 18.277 | | CPS3 |
| ATOM | 2561 | 0 | | | | 48.233 | | | CPS3 |
| MOTA | 2562 | N | ILE | 89 | 54.196 | | | | CPS3 |
| MOTA | 2563 | CA | ILE | 89 | 53.675 | 47.331 | | | CPS3 |
| MOTA | 2564 | CB | ILE | 89 | 54.406 | 45.966 | 19.939 | 1.00 17.33 | CF33 |
| | | | | | | | | | |

| ATOM | 2565 | CG2 | ILE | 89 | 54.146 | 45.145 | 21.217 | 1.00 18.20 | CPS3 |
|------|------|-----|-----|----------|--------|--------|--------|------------|------|
| ATOM | 2566 | CG1 | ILE | 89 | 53.938 | 45.192 | 18.696 | 1.00 18.54 | CPS3 |
| MOTA | 2567 | CD1 | | 89 | 54.805 | 43.948 | 18.365 | 1.00 18.01 | CPS3 |
| MOTA | 2568 | C | ILE | 89 | 53.775 | 47.829 | 21.450 | 1.00 18.41 | CPS3 |
| ATOM | 2569 | 0 | ILE | 89 | 54.749 | 48.465 | 21.832 | 1.00 18.45 | CPS3 |
| ATOM | 2570 | N | ILE | 90 | 52.737 | 47.539 | 22.221 | 1.00 19.17 | CPS3 |
| ATOM | 2571 | CA | ILE | 90 | 52.722 | 47.852 | 23.645 | 1.00 20.34 | CPS3 |
| ATOM | 2572 | CB | ILE | 90 | 51.485 | 48.700 | 24.062 | 1.00 20.34 | CPS3 |
| ATOM | 2572 | CG2 | | 90 | 51.364 | 48.738 | 25.608 | 1.00 21.03 | |
| ATOM | | | | | | | | 1.00 21.79 | CPS3 |
| | 2574 | CG1 | | 90 | 51.605 | 50.128 | 23.516 | | CPS3 |
| ATOM | 2575 | CD1 | | 90 | 52.787 | 50.918 | 24.079 | 1.00 22.03 | CPS3 |
| ATOM | 2576 | C | ILE | 90 | 52.618 | 46.483 | 24.314 | 1.00 20.90 | CPS3 |
| ATOM | 2577 | 0 | ILE | 90 | 51.722 | 45.704 | 23.994 | 1.00 22.15 | CPS3 |
| ATOM | 2578 | N | CYS | 91 | 53.557 | 46.177 | 25.208 | 1.00 21.50 | CPS3 |
| ATOM | 2579 | CA | CYS | 91 | 53.565 | 44.918 | 25.968 | 1.00 22.56 | CPS3 |
| ATOM | 2580 | CB | CYS | 91 | 54.379 | 43.834 | 25.252 | 1.00 22.42 | CPS3 |
| MOTA | 2581 | SG | CYS | 91 | 54.522 | 42.300 | 26.235 | 1.00 25.18 | CPS3 |
| MOTA | 2582 | C | CYS | 91 | 54.251 | 45.307 | 27.279 | 1.00 23.27 | CPS3 |
| MOTA | 2583 | 0 | CYS | 91 | 55.450 | 45.584 | 27.292 | 1.00 23.16 | CPS3 |
| MOTA | 2584 | N | THR | 92 | 53.500 | 45.337 | 28.372 | 1.00 26.40 | CPS3 |
| ATOM | 2585 | CA | THR | 92 | 54.076 | 45.784 | 29.638 | 1.00 28.79 | CPS3 |
| ATOM | 2586 | CB | THR | 92 | 52.983 | 46.002 | 30.713 | 1.00 29.85 | CPS3 |
| MOTA | 2587 | OG1 | THR | 92 | 52.347 | 44.760 | 31.033 | 1.00 31.45 | CPS3 |
| MOTA | 2588 | CG2 | THR | 92 | 51.934 | 46.993 | 30.195 | 1.00 30.30 | CPS3 |
| ATOM | 2589 | C | THR | 92 | 55.203 | 44.945 | 30.217 | 1.00 30.27 | CPS3 |
| ATOM | 2590 | 0 | THR | 92 | 55.787 | 45.313 | 31.237 | 1.00 29.37 | CPS3 |
| ATOM | 2591 | N | LYS | 93 | 55.520 | 43.828 | 29.571 | 1.00 30.96 | CPS3 |
| ATOM | 2592 | CA | LYS | 93 | 56.618 | 42.991 | 30.031 | 1.00 32.02 | CPS3 |
| MOTA | 2593 | CB | LYS | 93 | 56.521 | 41.608 | 29.397 | 1.00 33.43 | CPS3 |
| MOTA | 2594 | CG | LYS | 93 | 55.509 | 40.711 | 30.098 | 1.00 36.42 | CPS3 |
| ATOM | 2595 | CD | LYS | 93 | 55.253 | 39.426 | 29.337 | 1.00 38.18 | CPS3 |
| ATOM | 2596 | CE | LYS | 93 | 54.583 | 38.385 | 30.227 | 1.00 40.38 | CPS3 |
| ATOM | 2597 | NZ | LYS | 93 | 53.482 | 38.941 | 31.059 | 1.00 41.16 | CPS3 |
| ATOM | 2598 | C | LYS | 93 | 57.956 | 43.657 | 29.701 | 1.00 31.94 | CPS3 |
| MOTA | 2599 | Ō | LYS | 93 | 58.998 | 43.287 | 30.233 | 1.00 32.81 | CPS3 |
| MOTA | 2600 | N | LEU | 94 | 57.924 | 44.655 | 28.824 | 1.00 31.18 | CPS3 |
| ATOM | 2601 | CA | LEU | 94 | 59.139 | 45.378 | 28.473 | 1.00 30.06 | CPS3 |
| ATOM | 2602 | CB | LEU | 94 | 59.903 | 44.637 | | 1.00 31.03 | CPS3 |
| ATOM | 2603 | CG | LEU | 94 | 59.121 | 43.973 | 26.240 | 1.00 31.49 | CPS3 |
| ATOM | 2604 | | LEU | 94 | 58.228 | 44.977 | 25.551 | 1.00 33.11 | CPS3 |
| ATOM | 2605 | | LEU | 94 | 60.109 | 43.366 | 25.258 | 1.00 31.24 | CPS3 |
| ATOM | 2606 | C | LEU | 94 | 58.822 | 46.801 | 28.042 | 1.00 29.42 | CPS3 |
| ATOM | 2607 | | LEU | 94 | 57.657 | | | 1.00 28.23 | CPS3 |
| | | _ | SER | 95 | 59.852 | 47.618 | 27.841 | 1.00 28.87 | CPS3 |
| ATOM | 2608 | N | | | | | 27.423 | 1.00 29.31 | CPS3 |
| ATOM | 2609 | CA | SER | 95 05 | 59.616 | 48.993 | | 1.00 30.92 | CPS3 |
| ATOM | 2610 | CB | SER | 95 | 60.853 | 49.867 | | 1.00 30.32 | CPS3 |
| MOTA | 2611 | OG | SER | 95 | 60.671 | 51.106 | 26.950 | 1.00 31.74 | CPS3 |
| MOTA | 2612 | C | SER | 95 | 59.244 | 49.062 | 25.953 | | |
| MOTA | 2613 | 0 | SER | 95 | 59.835 | 48.376 | 25.127 | 1.00 27.86 | CPS3 |
| ATOM | 2614 | N | PRO | 96 | 58.269 | 49.914 | | 1.00 28.41 | CPS3 |
| ATOM | 2615 | CD | PRO | 96 | 57.504 | 50.793 | 26.516 | 1.00 29.30 | CPS3 |
| ATOM | 2616 | CA | PRO | 96 | 57.829 | 50.074 | 24.221 | 1.00 27.35 | CPS3 |
| MOTA | 2617 | CB | PRO | 96 | 56.749 | 51.155 | 24.312 | 1.00 28.52 | CPS3 |
| MOTA | 2618 | CG | PRO | 96 | 56.259 | 51.056 | 25.722 | 1.00 29.70 | CPS3 |
| MOTA | 2619 | С | PRO | 96 | 58.997 | 50.532 | | | CPS3 |
| ATOM | 2620 | 0 | PRO | 96 | 59.060 | 50.209 | 22.156 | | CPS3 |
| ATOM | 2621 | N | ALA | 97 | 59.922 | 51.283 | 23.940 | 1.00 26.21 | CPS3 |
| | | | | | | | | | |

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| MOTA | 2622 | CA | ALA | 97 | 61.073 | 51.804 | 23.203 | 1.00 26.00 | CPS3 |
|------|------|--------|-------|-----|----------|--------|--------|------------|------|
| ATOM | 2623 | CB | ALA | 97 | 61.821 | 52.824 | 24.060 | 1.00 28.49 | CPS3 |
| ATOM | 2624 | С | ALA | 97 | 62.031 | 50.709 | 22.744 | 1.00 25.63 | CPS3 |
| MOTA | 2625 | 0 | ALA | 97 | 62.858 | 50.921 | 21.858 | 1.00 24.95 | CPS3 |
| ATOM | 2626 | N | ALA | 98 | 61.916 | 49.532 | 23.342 | 1.00 24.02 | CPS3 |
| ATOM | 2627 | CA | ALA | 98 | 62.793 | 48.426 | 22.986 | 1.00 23.40 | CPS3 |
| ATOM | 2628 | CB | ALA | 98 | 63.054 | 47.574 | 24.215 | 1.00 25.00 | CPS3 |
| MOTA | 2629 | C | ALA | 98 | 62.208 | 47.553 | 21.880 | 1.00 22.32 | CPS3 |
| | | | ALA | 98 | 62.868 | 46.645 | 21.401 | 1.00 22.52 | CPS3 |
| ATOM | 2630 | O N | VAL | 99 | 60.979 | 47.842 | 21.460 | 1.00 21.24 | CPS3 |
| ATOM | 2631 | N | | | 60.330 | | | 1.00 21.24 | CPS3 |
| ATOM | 2632 | CA | VAL | 99 | | 47.004 | 20.457 | | CPS3 |
| MOTA | 2633 | CB | VAL | 99 | 58.965 | 46.511 | 20.982 | 1.00 19.94 | |
| ATOM | 2634 | | VAL | 99 | 58.383 | 45.474 | 20.027 | 1.00 21.36 | CPS3 |
| ATOM | 2635 | | VAL | 99 | 59.125 | 45.930 | 22.376 | 1.00 23.27 | CPS3 |
| MOTA | 2636 | C | LAV | 99 | 60.100 | 47.691 | 19.121 | 1.00 19.01 | CPS3 |
| MOTA | 2637 | 0 | VAL | 99 | 59.758 | 48.865 | 19.083 | 1.00 19.19 | CPS3 |
| MOTA | 2638 | N | HIS | 100 | 60.295 | 46.941 | 18.037 | 1.00 18.11 | CPS3 |
| ATOM | 2639 | CA | HIS | 100 | 60.080 | 47.439 | 16.685 | 1.00 19.23 | CPS3 |
| ATOM | 2640 | CB | HIS | 100 | 61.426 | 47.732 | 16.029 | 1.00 21.42 | CPS3 |
| MOTA | 2641 | CG | HIS | 100 | 62.233 | 48.753 | 16.772 | 1.00 24.13 | CPS3 |
| MOTA | 2642 | CD2 | HIS | 100 | 63.223 | 48.613 | 17.686 | 1.00 25.59 | CPS3 |
| ATOM | 2643 | ND1 | HIS | 100 | 62.007 | 50.105 | 16.654 | 1.00 25.95 | CPS3 |
| MOTA | 2644 | CE1 | HIS | 100 | 62.825 | 50.758 | 17.463 | 1.00 26.97 | CPS3 |
| MOTA | 2645 | NE2 | HIS | 100 | 63.572 | 49.874 | 18.100 | 1.00 26.97 | CPS3 |
| MOTA | 2646 | C | HIS | 100 | 59.343 | 46.348 | 15.919 | 1.00 18.08 | CPS3 |
| ATOM | 2647 | 0 | HIS | 100 | 59.707 | 45.178 | 16.027 | 1.00 17.62 | CPS3 |
| ATOM | 2648 | N | VAL | 101 | 58.313 | 46.731 | 15.161 | 1.00 17.20 | CPS3 |
| ATOM | 2649 | CA | LAV | 101 | 57.525 | 45.765 | 14.382 | 1.00 16.42 | CPS3 |
| MOTA | 2650 | CB | VAL | 101 | 56.149 | 45.472 | 15.080 | 1.00 16.35 | CPS3 |
| ATOM | 2651 | | VAL | 101 | 55.316 | 46.753 | 15.156 | 1.00 15.91 | CPS3 |
| ATOM | 2652 | | VAL | 101 | 55.364 | 44.375 | 14.330 | 1.00 17.27 | CPS3 |
| ATOM | 2653 | С | VAL | 101 | 57.244 | 46.312 | 12.982 | 1.00 16.80 | CPS3 |
| MOTA | 2654 | ō | VAL | 101 | 57.325 | 47.515 | 12.754 | 1.00 15.86 | CPS3 |
| ATOM | 2655 | N | SER | 102 | 56.948 | 45.414 | 12.046 | 1.00 16.94 | CPS3 |
| ATOM | 2656 | CA | SER | 102 | 56.554 | 45.816 | 10.694 | 1.00 17.40 | CPS3 |
| ATOM | 2657 | CB | SER | 102 | 57.733 | 45,889 | 9.723 | 1.00 18.13 | CPS3 |
| ATOM | 2658 | OG | SER | 102 | 57.255 | 46.343 | 8.454 | 1.00 19.88 | CPS3 |
| MOTA | 2659 | C | SER | 102 | 55.566 | 44.752 | 10.240 | 1.00 17.06 | CPS3 |
| ATOM | 2660 | 0 | SER | 102 | 55.738 | 43.569 | 10.531 | 1.00 16.38 | CPS3 |
| | 2661 | | ILE | 103 | 54.508 | 45.180 | 9.562 | 1.00 16.71 | CPS3 |
| ATOM | | N | | 103 | 53.476 | 44.259 | 9.109 | 1.00 16.77 | CPS3 |
| MOTA | 2662 | CA | ILE | | 52.138 | 44.533 | 9.851 | 1.00 19.32 | CPS3 |
| MOTA | 2663 | CB | ILE | 103 | | 43.538 | 9.386 | 1.00 20.27 | CPS3 |
| ATOM | 2664 | CG2 | | 103 | 51.062 | 44.398 | 11.366 | 1.00 18.63 | CPS3 |
| ATOM | 2665 | | LILE | 103 | 52.340 | | | 1.00 17.98 | CPS3 |
| ATOM | 2666 | | LILE | 103 | 51.099 | 44.754 | 12.195 | | CPS3 |
| MOTA | 2667 | C | ILE | 103 | 53.261 | 44.475 | 7.615 | 1.00 17.09 | CPS3 |
| ATOM | 2668 | 0 | ILE | 103 | 53.304 | 45.608 | 7.140 | 1.00 18.12 | CPS3 |
| ATOM | 2669 | N | THR | 104 | 53.038 | 43.390 | 6.880 | 1.00 18.52 | |
| MOTA | 2670 | CA | | 104 | 52.802 | 43.475 | 5.438 | 1.00 19.66 | CPS3 |
| MOTA | 2671 | CB | | 104 | 54.116 | 43.197 | 4.636 | 1.00 20.60 | CPS3 |
| ATOM | 2672 | OG: | 1 THR | 104 | 53.888 | 43.430 | 3.246 | 1.00 21.77 | CPS3 |
| ATOM | 2673 | CG: | 2 THR | 104 | 54.583 | 41.763 | 4.822 | 1.00 20.35 | CPS3 |
| ATOM | 2674 | C | THR | 104 | 51.694 | 42.494 | 5.020 | 1.00 20.81 | CPS3 |
| MOTA | 2675 | 0 | THR | 104 | 51.347 | 41.586 | 5.770 | 1.00 19.47 | CPS3 |
| ATOM | 2676 | N | HIS | 105 | 51.142 | 42.688 | 3.825 | 1.00 21.19 | CPS3 |
| ATOM | 2677 | CA | HIS | 105 | 50.066 | 41.838 | 3.320 | | CPS3 |
| ATOM | 2678 | CB | | 105 | 48.701 | 42.514 | 3.515 | 1.00 25.55 | CPS3 |
| | | | | | - | | | | |

| ATOM | 2679 | CG | HIS | 105 | 48.344 | 42.814 | 4.937 | 1.00 30.17 | CPS3 |
|--------------|------------------------------|--------|------------|------------|------------------|------------------|----------------|--------------------------|--------------|
| MOTA | 2680 | CD2 | HIS | 105 | 48.668 | 43.859 | 5.737 | 1.00 31.35 | CPS3 |
| MOTA | 2681 | ND1 | HIS | 105 | 47.507 | 42.008 | 5.676 | 1.00 31.23 | CPS3 |
| MOTA | 2682 | CEl | HIS | 105 | 47.327 | 42.544 | 6.872 | 1.00 33.22 | CPS3 |
| MOTA | 2683 | NE2 | HIS | 105 | 48.020 | 43.668 | 6.935 | 1.00 32.63 | CPS3 |
| ATOM | 2684 | C | HIS | 105 | 50.178 | 41.619 | 1.817 | 1.00 22.69 | CPS3 |
| MOTA | 2685 | 0 | HIS | 105 | 50.784 | 42.413 | 1.105 | 1.00 22.84 | CPS3 |
| MOTA | 2686 | N | THR | 106 | 49.565 | 40.536 | 1.359 | 1.00 24.26 | CPS3 |
| MOTA | 2687 | CA | THR | 106 | 49.426 | 40.244 | -0.066 | 1.00 25.12 | CPS3 |
| MOTA | 2688 | CB | THR | 106 | 50.338 | 39.107 | -0.598 | 1.00 25.65 | CPS3 |
| MOTA | 2689 | OGl | THR | 106 | 49.928 | 37.848 | -0.047 | 1.00 25.72 | CPS3 |
| MOTA | 2690 | CG2 | THR | 106 | 51.805 | 39.395 | -0.275 | 1.00 24.63 | CPS3 |
| MOTA | 2691 | С | THR | 106 | 47.970 | 39.769 | -0.097 | 1.00 25.84 | CPS3 |
| ATOM | 2692 | 0 | THR | 106 | 47.290 | 39.753 | 0.934 | 1.00 24.47 | CPS3 |
| ATOM | 2693 | N | ALA | 107 | 47.484 | 39.388 | -1.265 | 1.00 25.43 | CPS3 |
| ATOM | 2694 | CA | ALA | 107 | 46.108 | 38.937 | -1.362 | 1.00 26.46 | CPS3 |
| MOTA | 2695 | CB | ALA | 107 | 45.790 | 38.570 | -2.820 | 1.00 27.17 | CPS3 |
| ATOM | 2696 | C | ALA | 107 | 45.812 | 37.750 | -0.444 | 1.00 26.57 | CPS3 |
| ATOM | 2697 | 0 | ALA | 107 | 44.769 | 37.707 | 0.213 | 1.00 27.71 | CPS3 |
| ATOM | 2698 | N | GLU | 108 | 46.738 | 36.799 | -0.384 | 1.00 26.04 | CPS3 |
| ATOM | 2699 | CA | GLU | 108 | 46.542 | 35.594 | 0.404 | 1.00 25.62 | CPS3 |
| ATOM | 2700 | CB | GLU | 108 | 46.833 | 34.374 | -0.475 | 1.00 29.10 | CPS3 |
| MOTA | 2701 | CG | GLU | 108 | 46.172 | 34.475 | -1.846 | 1.00 35.56 | CPS3 |
| ATOM | 2702 | CD | GLU | 108 | 46.174 | 33.171 | -2.616 | 1.00 40.28 | CPS3 |
| ATOM | 2703 | OE1 | GLU | 108 | 47.145 | 32.395 | -2.485 | 1.00 42.87 | CPS3 |
| ATOM | 2704 | OE2 | GLU | 108 | 45.201 | 32.932 | -3.369 | 1.00 44.28 | CPS3 |
| ATOM | 2705 | C | GLU | 108 | 47.325 | 35.460 | 1.706 | 1.00 25.50 | CPS3 |
| ATOM | 2706 | 0 | GLU | 108 | 47.087 | 34.520 | 2.463 | 1.00 23.92 | CPS3 |
| MOTA | 270 7 | N | TYR | 109 | 48.239 | 36.389 | 1.978 | 1.00 23.47 | CPS3 |
| MOTA | 2708 | CA | TYR | 109 | 49.048 | 36.281 | 3.189 | 1.00 22.84 | CPS3 |
| MOTA | 2709 | CB | TYR | 109 | 50.471 | 35.833 | 2.822 | 1.00 23.00 | CPS3 |
| ATOM | 2710 | CG | TYR | 109 | 50.552 | 34.480 | 2.176 | 1.00 23.82 | CPS3 |
| ATOM | 2711 | CD1 | | 109 | 50.485 | 33.317 | 2.936 | 1.00 23.06 | CPS3 |
| MOTA | 2712 | CE1 | | 109 | 50.532 | 32.063 | 2.334 | 1.00 24.49 | CPS3 |
| MOTA | 2713 | CD2 | | 109 | 50.668 | 34.361 | 0.793 | 1.00 23.15 | CPS3 |
| MOTA | 2714 | CE2 | | 109 | 50.710 | 33.122 | 0.184 | 1.00 24.59 | CPS3 |
| ATOM | 2715 | CZ | TYR | 109 | 50.641 | 31.980 | 0.956 | 1.00 24.33 | CPS3 CPS3 |
| ATOM | 2716 | OH | TYR | 109 | 50.655 | 30.756 | 0.341 | 1.00 26.41 | CPS3 |
| ATOM | 2717 | C | TYR | 109 | 49.187 | 37.551 | 4.000 | 1.00 21.41 | CPS3 |
| ATOM | 2718 | 0 | TYR | 109 | 49.021 | 38.659 | 3.477 5.293 | 1.00 21.21 1.00 19.67 | CPS3 |
| ATOM | 2719 2720 | N | ALA ALA | 110 | 49.478 49.781 | 37.366 38.470 | 6.204 | 1.00 19.04 | CPS3 |
| MOTA | | CA | ALA | 110 110 | 49.781 | 38.470 | 7.334 | 1.00 19.04 | CPS3 |
| ATOM | 2721 | CB | | 110 | | 38.048 | 6.776 | 1.00 19.30 | CPS3 |
| ATOM | 2722 | C | ALA ALA | 110 | 51.137 51.375 | 36.861 | 6.985 | 1.00 10.30 | CPS3 |
| ATOM | 2723 2724 | N O | ALA | 111 | 52.038 | 38.997 | 7.014 | 1.00 18.04 | CPS3 |
| ATOM | | CA | ALA | 111 | 53.337 | 38.631 | 7.565 | 1.00 17.63 | CPS3 |
| MOTA MOTA | 2725 2726 | CB | ALA | 111 | 54.347 | 38.376 | 6.434 | 1.00 16.29 | CPS3 |
| | | C | ALA | 111 | 53.819 | 39.758 | 8.469 | 1.00 17.67 | CPS3 |
| ATOM ATOM | 272 7 272 8 | 0 | ALA | 111 | 53.404 | 40.903 | 8.312 | 1.00 18.51 | CPS3 |
| ATOM | 2729 | И | ALA | 112 | 54.672 | 39.424 | 9.428 | 1.00 16.56 | CPS3 |
| ATOM | 2730 | CA | ALA | 112 | 55.181 | 40.433 | 10.342 | 1.00 15.86 | CPS3 |
| ATOM | 2731 | CB | ALA | 112 | 54.203 | 40.636 | 11.489 | 1.00 15.01 | CPS3 |
| ATOM | 2732 | CB | ALA | 112 | 56.533 | 40.033 | 10.896 | 1.00 17.34 | CPS3 |
| ATOM | 2732 | 0 | ALA | 112 | 56.885 | 38.856 | 10.913 | 1.00 16.61 | CPS3 |
| ATOM | 2734 | N | GLN | 113 | 57.294 | 41.021 | 11.352 | 1.00 16.50 | CPS3 |
| ATOM | 2735 | CA | GLN | 113 | 58.591 | 40.732 | 11.952 | 1.00 18.53 | CPS3 |
| 111011 | 2.33 | | | | 20.251 | | | | |

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| MOTA | 2736 | CB | GLN | 113 | 59.735 | 40.962 | 10.956 | 1.00 18.24 | CPS3 |
|--------------|--------------|-----|-----|-----|--------|--------|--------|------------|------|
| MOTA | 2737 | CG | GLN | 113 | 59.926 | 42.406 | 10.544 | 1.00 22.84 | CPS3 |
| MOTA | 2738 | CD | GLN | 113 | 61.095 | 42.611 | 9.578 | 1.00 22.34 | |
| ATOM | 2739 | | GLN | 113 | | 43.738 | | | CPS3 |
| | | | | | 61.504 | | 9.326 | 1.00 28.00 | CPS3 |
| ATOM | 2740 | NE2 | | 113 | 61.624 | 41.521 | 9.033 | 1.00 28.26 | CPS3 |
| MOTA | 2741 | C | GLN | 113 | 58.724 | 41.667 | 13.144 | 1.00 16.72 | CPS3 |
| ATOM | 2742 | 0 | GLN | 113 | 58.108 | 42.728 | 13.182 | 1.00 16.09 | CPS3 |
| ATOM | 2743 | N | VAL | 114 | 59.513 | 41.252 | 14.124 | 1.00 17.10 | CPS3 |
| ATOM | 2744 | CA | VAL | 114 | 59.707 | 42.051 | 15.329 | 1.00 17.04 | CPS3 |
| MOTA | 2745 | CB | VAL | 114 | 58.882 | 41.484 | 16.538 | 1.00 17.59 | CPS3 |
| MOTA | 2746 | CG1 | VAL | 114 | 59.307 | 42.160 | 17.853 | 1.00 17.11 | CPS3 |
| ATOM | 2747 | CG2 | VAL | 114 | 57.392 | 41.703 | 16.320 | 1.00 16.91 | CPS3 |
| ATOM | 2748 | С | VAL | 114 | 61.173 | 41.971 | 15.710 | 1.00 18.24 | CPS3 |
| ATOM | 2749 | ō | VAL | 114 | 61.826 | 40.948 | 15.493 | 1.00 16.19 | CPS3 |
| MOTA | 2750 | N | VAL | 115 | 61.691 | 43.068 | 16.251 | 1.00 18.16 | CPS3 |
| MOTA | 2751 | CA | VAL | 115 | 63.053 | 43.072 | 16.231 | | |
| | | | | | | | | 1.00 19.36 | CPS3 |
| MOTA | 2752 | CB | VAL | 115 | 64.021 | 43.925 | 15.920 | 1.00 20.69 | CPS3 |
| MOTA | 2753 | | VAL | 115 | 65.394 | 44.014 | 16.637 | 1.00 20.85 | CPS3 |
| ATOM | 2754 | | VAL | 115 | 64.184 | 43.305 | 14.529 | 1.00 18.29 | CPS3 |
| MOTA | 2755 | C | VAL | 115 | 62.916 | 43.691 | 18.148 | 1.00 20.16 | CPS3 |
| ATOM | 2756 | 0 | VAL | 115 | 62.268 | 44.728 | 18.309 | 1.00 21.78 | CPS3 |
| MOTA | 2757 | N | ILE | 116 | 63.463 | 43.018 | 19.152 | 1.00 20.33 | CPS3 |
| MOTA | 2758 | CA | ILE | 116 | 63.438 | 43.527 | 20.517 | 1.00 21.08 | CPS3 |
| ATOM | 2759 | CB | ILE | 116 | 62.911 | 42.491 | 21.517 | 1.00 21.66 | CPS3 |
| MOTA | 2760 | CG2 | ILE | 116 | 63.081 | 43.042 | 22.960 | 1.00 21.13 | CPS3 |
| ATOM | 2761 | CG1 | ILE | 116 | 61.439 | 42.174 | 21.215 | 1.00 21.09 | CPS3 |
| ATOM | 2762 | CD1 | | 116 | 60.806 | 41.091 | 22.118 | 1.00 19.60 | CPS3 |
| MOTA | 2763 | C | ILE | 116 | 64.881 | 43.835 | 20.885 | 1.00 24.39 | CPS3 |
| MOTA | 2764 | ō | ILE | 116 | 65.764 | 42.993 | 20.697 | 1.00 22.81 | CPS3 |
| MOTA | 2765 | N | GLU | 117 | 65.131 | 45.041 | 21.381 | 1.00 26.58 | CPS3 |
| MOTA | 2766 | CA | GLU | 117 | 66.487 | 45.410 | 21.767 | 1.00 20.30 | CPS3 |
| | 276 7 | CB | GLU | 117 | 66.824 | 46.834 | 21.346 | 1.00 32.50 | CPS3 |
| ATOM ATOM | 2768 | CG | GLU | 117 | | | 19.901 | | CPS3 |
| | | | | | 66.641 | 47.178 | | 1.00 37.84 | |
| MOTA | 2769 | CD | GLU | 117 | 67.052 | 48.616 | 19.638 | 1.00 40.98 | CPS3 |
| MOTA | 2770 | | GLU | 117 | 68.271 | 48.872 | 19.516 | 1.00 42.89 | CPS3 |
| MOTA | 2771 | | GLU | 117 | 66.160 | 49.491 | 19.578 | 1.00 43.15 | CPS3 |
| MOTA | 2772 | C | GLU | 117 | 66.653 | 45.367 | 23.275 | 1.00 33.73 | CPS3 |
| MOTA | 2773 | 0 | GLU | 117 | 65.679 | 45.454 | 24.026 | 1.00 33.05 | CPS3 |
| ATOM | 2774 | N | ARG | 118 | 67.904 | 45.244 | 23.708 | 1.00 37.38 | CPS3 |
| ATOM | 2775 | CA | ARG | 118 | 68.224 | 45.267 | 25.124 | 1.00 41.10 | CPS3 |
| MOTA | 2776 | CB | ARG | 118 | 69.512 | 44.496 | 25.407 | 1.00 42.40 | CPS3 |
| MOTA | 2777 | CG | ARG | 118 | 69.311 | 43.126 | 26.025 | 1.00 44.67 | CPS3 |
| MOTA | 2778 | CD | ARG | 118 | 70.649 | 42.566 | 26.483 | 1.00 45.83 | CPS3 |
| ATOM | 2779 | NE | ARG | 118 | 71.614 | 42.542 | 25.389 | 1.00 47.03 | CPS3 |
| MOTA | 2780 | CZ | ARG | 118 | 71.609 | 41.652 | 24.402 | 1.00 47.03 | CPS3 |
| ATOM | 2781 | | ARG | 118 | 70.690 | 40.694 | 24.367 | 1.00 46.54 | CPS3 |
| ATOM | 2782 | | ARG | 118 | 72.520 | 41.729 | 23.446 | 1.00 46.88 | CPS3 |
| | | C | | | | | 25.399 | 1.00 42.76 | CPS3 |
| ATOM | 2783 | | ARG | 118 | 68.452 | 46.744 | | | CPS3 |
| ATOM | 2784 | 0 | ARG | 118 | 69.227 | 47.392 | 24.697 | 1.00 44.45 | |
| ATOM | 2785 | N | LEU | 119 | 67.765 | 47.289 | 26.392 | 1.00 45.54 | CPS3 |
| MOTA | 2786 | CA | LEU | 119 | 67.928 | 48.699 | 26.722 | 1.00 47.93 | CPS3 |
| ATOM | 2787 | CB | LEU | 119 | 66.563 | 49.328 | 27.014 | 1.00 48.16 | CPS3 |
| ATOM | 2788 | CG | LEU | 119 | 65.944 | 50.257 | 25.963 | 1.00 47.88 | CPS3 |
| ATOM | 2789 | CD1 | LEU | 119 | 66.182 | 49.739 | 24.548 | 1.00 47.81 | CPS3 |
| ATOM | 2790 | CD2 | LEU | 119 | 64.460 | 50.385 | 26.260 | 1.00 47.26 | CPS3 |
| ATOM | 2791 | Ç | LEU | 119 | 68.845 | 48.862 | 27.928 | 1.00 49.49 | CPS3 |
| MOTA | 2792 | OT1 | LEU | 119 | 70.001 | 49.296 | 27.728 | 1.00 50.38 | CPS3 |
| | | | | | | | | | |

| MOTA | 2793 | OT2 | | 119 | 68.399 | 48.537 | 29.052 | 1.00 51.04 | CPS3 |
|------|------|-----|-----|--------|--------|--------|--------|------------|--------------|
| ATOM | 2794 | С | GLY | 0 | 33.524 | 21.933 | 24.405 | 1.00 41.93 | CPS4 |
| ATOM | 2795 | 0 | GLY | 0 | 33.109 | 21.427 | 23.356 | 1.00 43.93 | CPS4 |
| ATOM | 2796 | N | GLY | 0 | 35.967 | 22.519 | 24.212 | 1.00 43.67 | CPS4 |
| MOTA | 2797 | CA | GLY | 0 | 34.574 | 23.033 | 24.374 | 1.00 42.80 | CPS4 |
| ATOM | 2798 | N | GLY | 1 | 33.089 | 21.565 | 25.607 | 1.00 38.91 | CPS4 |
| ATOM | 2799 | CA | GLY | 1 | 32.082 | 20.530 | 25.746 | 1.00 34.29 | CPS4 |
| MOTA | 2800 | C | GLY | 1 | 30.697 | 21.104 | 25.995 | 1.00 31.42 | CPS4 |
| ATOM | 2801 | 0 | GLY | 1 | 29.713 | 20.369 | 26.051 | 1.00 30.75 | CPS4 |
| ATOM | 2802 | N | ILE | 2 | 30.618 | 22.419 | 26.172 | 1.00 28.92 | CPS4 |
| ATOM | 2803 | CA | ILE | 2 | 29.328 | 23.068 | 26.405 | 1.00 26.32 | CPS4 |
| ATOM | 2804 | CB | ILE | 2 | 29.309 | 23.809 | 27.765 | 1.00 26.73 | CPS4 |
| ATOM | 2805 | CG2 | | 2 | 28.044 | 24.683 | 27.891 | 1.00 24.71 | CPS4 |
| ATOM | 2806 | CG1 | | 2 | 29.358 | 22.779 | 28.896 | 1.00 27.21 | CPS4 |
| ATOM | 2807 | CD1 | | 2 | 29.417 | 23.387 | 30.265 | 1.00 27.21 | CPS4 |
| ATOM | 2808 | C | ILE | 2 | 29.028 | 24.043 | 25.277 | 1.00 25.17 | CPS4 |
| ATOM | 2809 | 0 | ILE | 2 | 29.861 | 24.874 | 24.922 | 1.00 24.41 | CPS4 |
| MOTA | 2810 | | TYR | 3 | 27.839 | 23.910 | 24.703 | 1.00 24.41 | |
| | | N | TYR | 3 | | | 23.606 | 1.00 24.67 | CPS4 CPS4 |
| ATOM | 2811 | CA | | | 27.389 | 24.765 | | • | |
| ATOM | 2812 | CB | TYR | 3 | 26.260 | 24.071 | 22.850 | 1.00 27.01 | CPS4 |
| ATOM | 2813 | CG | TYR | 3 | 25.726 | 24.865 | 21.681 | 1.00 29.25 | CPS4 |
| ATOM | 2814 | | TYR | 3 | 26.385 | 24.861 | 20.452 | 1.00 31.33 | CPS4 |
| ATOM | 2815 | | TYR | 3 | 25.916 | 25.616 | 19.379 | 1.00 33.16 | CPS4 |
| ATOM | 2816 | | TYR | 3 | 24.579 | 25.645 | 21.811 | 1.00 31.21 | CPS4 |
| ATOM | 2817 | CE2 | | 3 | 24.101 | 26.409 | 20.740 | 1.00 32.57 | CPS4 |
| MOTA | 2818 | CZ | TYR | 3 | 24.776 | 26.388 | 19.530 | 1.00 34.44 | CPS4 |
| ATOM | 2819 | OH | TYR | 3 | 24.328 | 27.148 | 18.473 | 1.00 36.34 | CPS4 |
| MOTA | 2820 | С | TYR | 3 | 26.881 | 26.103 | 24.151 | 1.00 23.47 | CPS4 |
| ATOM | 2821 | 0 | TYR | 3 | 27.167 | 27.175 | 23.609 | 1.00 22.30 | CPS4 |
| ATOM | 2822 | N | GLY | 4 | 26.111 | 26.036 | 25.226 | 1.00 21.50 | CPS4 |
| MOTA | 2823 | CA | GLY | 4 | 25.597 | 27.262 | 25.802 | 1.00 20.66 | CPS4 |
| ATOM | 2824 | C | GLY | 4 | 24.775 | 26.974 | 27.036 | 1.00 18.15 | CPS4 |
| MOTA | 2825 | 0 | GLY | 4 | 24.397 | 25.824 | 27.275 | 1.00 17.40 | CPS4 |
| MOTA | 2826 | N | ILE | 5 | 24.519 | 28.019 | 27.827 | 1.00 17.22 | CPS4 |
| ATOM | 2827 | CA | ILE | 5 | 23.725 | 27.874 | 29.039 | 1.00 16.89 | CPS4 |
| MOTA | 2828 | CB | ILE | 5 | 24.585 | 27.961 | 30.311 | 1.00 17.48 | CPS4 |
| ATOM | 2829 | CG2 | ILE | 5 | 25.700 | 26.921 | 30.241 | 1.00 16.93 | CPS4 |
| ATOM | 2830 | CG1 | ILE | 5 | 25.166 | 29.374 | 30.472 | 1.00 18.44 | CPS4 |
| MOTA | 2831 | CD1 | ILE | 5 | 26.002 | 29.560 | 31.716 | 1.00 17.67 | CPS4 |
| ATOM | 2832 | C | ILE | 5 | 22.673 | 28.972 | 29.079 | 1.00 16.76 | CPS4 |
| ATOM | 2833 | 0 | ILE | 5 | 22.831 | 30.024 | 28.457 | 1.00 17.03 | CPS4 |
| ATOM | 2834 | N | GLY | 6 | 21.601 | 28.723 | 29.816 | 1.00 16.72 | CPS4 |
| ATOM | 2835 | CA | GLY | 6 | 20.537 | 29.702 | 29.894 | 1.00 17.09 | CPS4 |
| ATOM | 2836 | C | GLY | 6 | 19.874 | 29.687 | 31.246 | 1.00 17.29 | CPS4 |
| ATOM | 2837 | Õ | GLY | 6 | 19.730 | 28.638 | 31.869 | 1.00 17.78 | CPS4 |
| ATOM | 2838 | N | LEU | 7 | 19.485 | 30.874 | 31.703 | 1.00 16.88 | CPS4 |
| ATOM | 2839 | CA | LEU | 7 | 18.825 | 31.033 | 32.990 | 1.00 17.08 | CPS4 |
| ATOM | 2840 | CB | LEU | 7 | 19.803 | 31.622 | 34.006 | 1.00 18.18 | CPS4 |
| | 2841 | CG | LEU | 7 | 19.251 | 31.984 | 35.389 | 1.00 18.23 | CPS4 |
| MOTA | | | | | | | 36.200 | 1.00 17.58 | CPS4 |
| ATOM | 2842 | | LEU | 7 7 | 18.988 | 30.707 | 36.200 | 1.00 17.38 | CPS4 |
| ATOM | 2843 | | LEU | | 20.282 | 32.875 | | 1.00 17.74 | CPS4 |
| ATOM | 2844 | C | LEU | 7 | 17.660 | 31.998 | 32.817 | | CPS4 |
| ATOM | 2845 | 0 | LEU | 7 | 17.775 | 32.976 | 32.082 | 1.00 18.10 | |
| MOTA | 2846 | N | ASP | 8 | 16.539 | 31.712 | 33.471 | 1.00 18.02 | CPS4 |
| ATOM | 2847 | CA | ASP | 8 | 15.394 | 32.612 | 33.413 | 1.00 18.03 | CPS4 |
| MOTA | 2848 | CB | ASP | 8 | 14.426 | 32.202 | 32.305 | 1.00 20.37 | CPS4 |
| ATOM | 2849 | CG | ASP | 8 | 13.195 | 33.108 | 32.250 | 1.00 22.41 | CPS4 |

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| MOTA | 2850 | OD1 | ASP | 8 | 12.194 | 32.814 | 32.922 | 1.00 25.67 | CPS4 |
|------|------|-----|-----|----|----------------|--------|--------|------------|--------------|
| ATOM | 2851 | OD2 | ASP | 8 | 13.245 | 34.131 | 31.551 | 1.00 24.39 | CPS4 |
| MOTA | 2852 | C | ASP | 8 | 14.645 | 32.619 | 34.732 | 1.00 19.46 | CPS4 |
| ATOM | 2853 | 0 | ASP | 8 | 14.490 | 31.574 | 35.363 | 1.00 17.36 | CPS4 |
| ATOM | 2854 | N | ILE | 9 | 14.239 | 33.806 | 35.183 | 1.00 18.34 | CPS4 |
| ATOM | 2855 | CA | ILE | 9 | 13.420 | 33.898 | 36.376 | 1.00 19.60 | CPS4 |
| ATOM | 2856 | CB | ILE | 9 | 14.086 | 34.711 | 37.519 | 1.00 19.76 | CPS4 |
| MOTA | 2857 | CG2 | | 9 | 13.133 | 34.805 | 38.700 | 1.00 21.48 | CPS4 |
| ATOM | 2858 | CGI | | 9 | 15.366 | 34.012 | 37.982 | 1.00 20.86 | CPS4 |
| ATOM | 2859 | CD1 | | 9 | 16.146 | 34.790 | 39.050 | 1.00 20.88 | CPS4 |
| ATOM | 2860 | CDI | ILE | 9 | 12.171 | 34.623 | | | |
| | | | | | | | 35.878 | 1.00 20.38 | CPS4 |
| ATOM | 2861 | 0 | ILE | 9 | 12.277 | 35.629 | 35.167 | 1.00 20.64 | CPS4 |
| ATOM | 2862 | N | THR | 10 | 10.996 | 34.086 | 36.205 | 1.00 19.99 | CPS4 |
| ATOM | 2863 | CA. | THR | 10 | 9.749 | 34.700 | 35.781 | 1.00 20.69 | CPS4 |
| ATOM | 2864 | CB | THR | 10 | 8.999 | 33.803 | 34.777 | 1.00 21.55 | CPS4 |
| ATOM | 2865 | | THR | 10 | 9.775 | 33.679 | 33.572 | 1.00 23.30 | CPS4 |
| ATOM | 2866 | CG2 | | 10 | 7.639 | 34.414 | 34.433 | 1.00 23.59 | CPS4 |
| MOTA | 2867 | С | THR | 10 | 8.833 | 34.990 | 36.970 | 1.00 20.24 | CPS4 |
| MOTA | 2868 | 0 | THR | 10 | 8.677 | 34.166 | 37.865 | 1.00 18.97 | CPS4 |
| MOTA | 2869 | И | GLU | 11 | 8.233 | 36.173 | 36.971 | 1.00 21.51 | CPS4 |
| MOTA | 2870 | CA | GLU | 11 | 7.321 | 36.560 | 38.045 | 1.00 23.43 | CPS4 |
| ATOM | 2871 | CB | GLU | 11 | 7.180 | 38.085 | 38.070 | 1.00 26.54 | CPS4 |
| ATOM | 2872 | CG | GLU | 11 | 6.189 | 38.601 | 39.095 | 1.00 28.77 | CPS4 |
| MOTA | 2873 | CD | GLU | 11 | 6.072 | 40.116 | 39.097 | 1.00 30.52 | CPS4 |
| ATOM | 2874 | OE1 | GLU | 11 | 6.416 | 40.744 | 38.078 | 1.00 29.88 | CPS4 |
| MOTA | 2875 | OE2 | GLU | 11 | 5.615 | 40.675 | 40.118 | 1.00 33.84 | CPS4 |
| ATOM | 2876 | C | GLU | 11 | 5.959 | 35.906 | 37.791 | 1.00 24.01 | CPS4 |
| ATOM | 2877 | 0 | GLU | 11 | 5.344 | 36.137 | 36.750 | 1.00 23.79 | CPS4 |
| MOTA | 2878 | N | LEU | 12 | 5.482 | 35.092 | 38.730 | 1.00 23.66 | CPS4 |
| ATOM | 2879 | CA | LEU | 12 | 4.191 | 34.416 | 38.556 | 1.00 25.00 | CPS4 |
| MOTA | 2880 | CB | LEU | 12 | 3.804 | 33.609 | 39.798 | 1.00 26.31 | CP\$4 |
| ATOM | 2881 | CG | LEU | 12 | 4.621 | 32.386 | 40.208 | 1.00 31.01 | CPS4 |
| ATOM | 2882 | CD1 | LEU | 12 | 3.877 | 31.679 | 41.347 | 1.00 31.83 | CPS4 |
| MOTA | 2883 | CD2 | LEU | 12 | 4.808 | 31.435 | 39.028 | 1.00 32.20 | CPS4 |
| ATOM | 2884 | C | LEU | 12 | 3.044 | 35.391 | 38.253 | 1.00 24.98 | CPS4 |
| ATOM | 2885 | 0 | LEU | 12 | 2.196 | 35.107 | 37.412 | 1.00 24.51 | CPS4 |
| ATOM | 2886 | N | ALA | 13 | 3.019 | 36.524 | 38.950 | 1.00 25.40 | CPS4 |
| ATOM | 2887 | CA | ALA | 13 | 1.968 | 37.527 | 38.744 | 1.00 25.67 | CPS4 |
| ATOM | 2888 | CB | ALA | 13 | 2.157 | 38.691 | 39.702 | 1.00 28.52 | CPS4 |
| ATOM | 2889 | C | ALA | 13 | 1.939 | 38.044 | 37.314 | 1.00 26.33 | CPS4 |
| MOTA | 2890 | ō | ALA | 13 | 0.871 | 38.344 | 36.781 | 1.00 26.54 | CPS4 |
| ATOM | 2891 | N | ARG | 14 | 3.107 | 38.152 | 36.688 | 1.00 24.68 | CPS4 |
| ATOM | 2892 | CA | ARG | 14 | 3.179 | 38.644 | 35.318 | 1.00 26.32 | CPS4 |
| ATOM | 2893 | CB | ARG | 14 | 4.644 | 38.886 | 34.925 | 1.00 28.73 | CPS4 |
| ATOM | 2894 | CG | ARG | 14 | 4.859 | 39.331 | 33.482 | 1.00 34.36 | CPS4 |
| MOTA | 2895 | CD | ARG | 14 | 6.328 | 39.142 | 33.058 | 1.00 37.57 | CPS4 |
| | | | ARG | | 6.497 | 39.219 | 31.608 | 1.00 41.82 | CPS4 |
| ATOM | 2896 | NE | | 14 | | 39.219 | 30.947 | 1.00 42.56 | CPS4 |
| ATOM | 2897 | CZ | ARG | 14 | 7.529 8.491 | | | 1.00 43.08 | CPS4 |
| MOTA | 2898 | | ARG | 14 | | 38.070 | 31.603 | | CPS4 |
| ATOM | 2899 | | ARG | 14 | 7.597 | 38.817 | 29.627 | 1.00 44.77 | CPS4 CPS4 |
| MOTA | 2900 | С | ARG | 14 | 2.533 | 37.633 | 34.370 | 1.00 25.53 | |
| MOTA | 2901 | 0 | ARG | 14 | 1.783 | 38.001 | 33.465 | 1.00 25.68 | CPS4 |
| ATOM | 2902 | N | ILE | 15 | 2.832 | 36.357 | 34.585 | 1.00 24.70 | CPS4 |
| MOTA | 2903 | CA | ILE | 15 | 2.278 | 35.284 | 33.763 | 1.00 25.07 | CPS4 |
| ATOM | 2904 | CB | ILE | 15 | 2.884 | 33.920 | 34.153 | 1.00 24.95 | CPS4 |
| MOTA | 2905 | | ILE | 15 | 2.169 | 32.782 | 33.390 | 1.00 24.82 | CPS4 |
| MOTA | 2906 | CG1 | ILE | 15 | 4.382 | 33.913 | 33.849 | 1.00 24.68 | CPS4 |

| ATOM | 2907 | CD1 | ILE | 15 | 4.714 | 33.980 | 32.358 | 1.00 27.32 | CPS4 |
|------|------|-----|-----|----|---------|-------------|--------|------------|------|
| MOTA | 2908 | C | ILE | 15 | 0.766 | 35.200 | 33.950 | 1.00 26.73 | CPS4 |
| MOTA | 2909 | 0 | ILE | 15 | 0.009 | 34.983 | 32.993 | 1.00 25.85 | CPS4 |
| ATOM | 2910 | N | ALA | 16 | 0.324 | 35.352 | 35.193 | 1.00 26.46 | CPS4 |
| MOTA | 2911 | CA | ALA | 16 | -1.104 | 35.273 | 35.469 | 1.00 27.92 | CPS4 |
| ATOM | 2912 | CB | ALA | 16 | -1.355 | 35.318 | 36.975 | 1.00 28.33 | CPS4 |
| ATOM | 2913 | C | ALA | 16 | -1.823 | 36.423 | 34.774 | 1.00 29.55 | CPS4 |
| MOTA | 2914 | 0 | ALA | 16 | -2.928 | 36.252 | 34.240 | 1.00 29.47 | CPS4 |
| ATOM | 2915 | N | SER | 17 | -1.191 | 37.592 | 34.772 | 1.00 29.18 | CPS4 |
| ATOM | 2916 | CA | SER | 17 | -1.783 | 38.760 | 34.136 | 1.00 31.51 | CPS4 |
| MOTA | 2917 | CB | SER | 17 | -0.944 | 40.000 | 34.429 | 1.00 33.05 | CPS4 |
| ATOM | 2918 | OG | SER | 17 | -1.421 | 41.104 | 33.672 | 1.00 39.63 | CPS4 |
| ATOM | 2919 | C | SER | 17 | -1.922 | 38.574 | 32.624 | 1.00 32.08 | CPS4 |
| MOTA | 2920 | 0 | SER | 17 | -2.974 | 38.874 | 32.045 | 1.00 31.35 | CPS4 |
| ATOM | 2921 | N | MET | 18 | -0.871 | 38.078 | 31.982 | 1.00 31.52 | CPS4 |
| ATOM | 2922 | CA | MET | 18 | -0.912 | 37.868 | 30.540 | 1.00 32.75 | CPS4 |
| MOTA | 2923 | CB | MET | 18 | 0.469 | 37.482 | 30.008 | 1.00 34.03 | CPS4 |
| ATOM | 2924 | CG | MET | 18 | 1.504 | 38.580 | 30.147 | 1.00 38.00 | CPS4 |
| ATOM | 2925 | SD | MET | 18 | 3.076 | 38.170 | 29.360 | 1.00 41.64 | CPS4 |
| ATOM | 2926 | CE | MET | 18 | 3.866 | 37.225 | 30.666 | 1.00 38.75 | CPS4 |
| ATOM | 2927 | C | MET | 18 | -1.917 | 36.793 | 30.156 | 1.00 32.75 | CPS4 |
| ATOM | 2928 | ō | MET | 18 | -2.689 | 36.971 | 29.215 | 1.00 32.74 | CPS4 |
| ATOM | 2929 | N | ALA | 19 | -1.906 | 35.686 | 30.893 | 1.00 33.01 | CPS4 |
| ATOM | 2930 | CA | ALA | 19 | -2.801 | 34.569 | 30.618 | 1.00 34.57 | CPS4 |
| ATOM | 2931 | CB | ALA | 19 | -2.458 | 33.384 | 31.515 | 1.00 34.76 | CPS4 |
| ATOM | 2932 | C | ALA | 19 | -4.262 | 34.944 | 30.793 | 1.00 36.04 | CPS4 |
| MOTA | 2933 | Ō | ALA | 19 | -5.140 | 34.338 | 30.176 | 1.00 36.08 | CPS4 |
| ATOM | 2934 | N | GLY | 20 | -4.523 | 35.942 | 31.630 | 1.00 36.62 | CPS4 |
| ATOM | 2935 | CA | GLY | 20 | -5.896 | 36.360 | 31.852 | 1.00 38.42 | CPS4 |
| ATOM | 2936 | C | GLY | 20 | -6.379 | 37.392 | 30.850 | 1.00 38.57 | CPS4 |
| MOTA | 2937 | ō | GLY | 20 | -7.560 | 37.437 | 30.511 | 1.00 38.87 | CPS4 |
| ATOM | 2938 | N | ARG | 21 | -5.460 | 38.210 | 30.355 | 1.00 38.64 | CPS4 |
| ATOM | 2939 | CA | ARG | 21 | -5.813 | 39.261 | 29.417 | 1.00 39.87 | CPS4 |
| MOTA | 2940 | CB | ARG | 21 | -4.944 | 40.489 | 29.695 | 1.00 42.18 | CPS4 |
| MOTA | 2941 | CG | ARG | 21 | -4.955 | 40.913 | 31.156 | 1.00 47.12 | CPS4 |
| ATOM | 2942 | CD | ARG | 21 | -4.162 | 42.195 | 31.381 | 1.00 50.94 | CPS4 |
| MOTA | 2943 | NE | ARG | 21 | -4.149 | 42.582 | 32.792 | 1.00 55.15 | CPS4 |
| ATOM | 2944 | CZ | ARG | 21 | -3.691 | 43.746 | 33.252 | 1.00 56.93 | CPS4 |
| ATOM | 2945 | | ARG | 21 | -3.721 | 44.005 | 34.554 | 1.00 57.41 | CPS4 |
| MOTA | 2946 | | ARG | 21 | -3.211 | 44.656 | 32.412 | 1.00 57.54 | CPS4 |
| MOTA | 2947 | C | ARG | 21 | -5.699 | 38.879 | 27.942 | 1.00 39.28 | CPS4 |
| ATOM | 2948 | ō | ARG | 21 | -6.223 | 39.587 | 27.080 | 1.00 39.05 | CPS4 |
| ATOM | | N | GLN | 22 | | 37.764 | | 1.00 37.77 | CPS4 |
| MOTA | 2950 | CA | GLN | 22 | -4.823 | 37.311 | 26.276 | 1.00 37.67 | CPS4 |
| ATOM | 2951 | CB | GLN | 22 | -3.325 | 37.254 | 25.979 | 1.00 36.76 | CPS4 |
| ATOM | 2952 | CG | GLN | 22 | -2.634 | 38.603 | 26.038 | 1.00 40.23 | CPS4 |
| MOTA | 2953 | | GLN | 22 | -1.135 | 38.490 | 25.871 | 1.00 41.78 | CPS4 |
| ATOM | 2954 | | GLN | 22 | -0.652 | 37.746 | 25.018 | 1.00 43.79 | CPS4 |
| ATOM | 2955 | | GLN | 22 | -0.389 | 39.236 | 26.677 | 1.00 42.68 | CPS4 |
| ATOM | 2956 | C | GLN | 22 | -5.441 | 35.947 | 25.997 | 1.00 37.08 | CPS4 |
| ATOM | 2957 | ō | GLN | 22 | -5.004 | 34.936 | 26.560 | 1.00 37.84 | CPS4 |
| ATOM | 2958 | N | LYS | 23 | -6.431 | 35.910 | 25.106 | 1.00 34.80 | CPS4 |
| ATOM | 2959 | CA | LYS | 23 | -7.114 | 34.661 | 24.781 | 1.00 34.70 | CPS4 |
| ATOM | 2960 | CB | LYS | 23 | -8.133 | 34.862 | 23.641 | 1.00 35.14 | CPS4 |
| ATOM | 2961 | CG | LYS | 23 | -9.497 | 35.362 | 24.090 | 1.00 37.14 | CPS4 |
| ATOM | 2962 | CD | LYS | 23 | -10.626 | 34.901 | 23.159 | 1.00 37.66 | CPS4 |
| MOTA | 2963 | CE | LYS | 23 | -10.491 | 35.444 | 21.745 | 1.00 36.38 | CPS4 |
| | 2505 | | | | | · · | | | |

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| N COM | 2064 | 1777 | T 370 | 2.2 | 11 722 | 25 177 | 22 22 | | ana. |
|-------|------|------|-------|-----|---------|--------|--------|------------|------|
| ATOM | 2964 | NZ | LYS | 23 | -11.732 | 35.177 | 20.937 | 1.00 32.97 | CPS4 |
| MOTA | 2965 | | LYS | 23 | -6.211 | 33.491 | 24.403 | 1.00 32.65 | CPS4 |
| ATOM | 2966 | | LYS | 23 | -6.488 | 32.356 | 24.775 | 1.00 33.18 | CPS4 |
| ATOM | 2967 | N | ARG | 24 | -5.143 | 33.754 | 23.659 | 1.00 31.45 | CPS4 |
| ATOM | 2968 | CA | ARG | 24 | -4.265 | 32.662 | 23.227 | 1.00 31.24 | CPS4 |
| ATOM | 2969 | CB _ | ARG | 24 | -4.159 | 32.665 | 21.691 | 1.00 32.20 | CPS4 |
| MOTA | 2970 | CG | ARG | 24 | -5.218 | 31.798 | 20.979 | 1.00 34.37 | CPS4 |
| ATOM | 2971 | CD | ARG | 24 | -6.636 | 32.172 | 21.379 | 1.00 34.60 | CPS4 |
| ATOM | 2972 | NE . | ARG | 24 | -7.668 | 31.404 | 20.672 | 1.00 34.87 | CPS4 |
| MOTA | 2973 | CZ | ARG | 24 | -8.339 | 30.379 | 21.191 | 1.00 34.53 | CPS4 |
| ATOM | 2974 | NH1 | | 24 | -8.095 | 29.976 | 22.428 | 1.00 33.25 | CPS4 |
| ATOM | 2975 | | ARG | 24 | -9.281 | 29.770 | 20.478 | 1.00 35.11 | CPS4 |
| MOTA | 2976 | C | ARG | 24 | -2.864 | 32.603 | 23.832 | 1.00 29.23 | CPS4 |
| | | | ARG | | -1.967 | 31.992 | 23.032 | 1.00 29.23 | |
| ATOM | 2977 | 0 | | 24 | | | | | CPS4 |
| MOTA | 2978 | N | PHE | 25 | -2.669 | 33.208 | 24.995 | 1.00 27.93 | CPS4 |
| ATOM | 2979 | CA | PHE | 25 | -1.339 | 33.186 | 25.604 | 1.00 26.76 | CPS4 |
| MOTA | 2980 | CB | PHE | 25 | -1.339 | 33.979 | 26.916 | 1.00 27.25 | CPS4 |
| ATOM | 2981 | CG | PHE | 25 | 0.016 | 34.068 | 27.564 | 1.00 28.14 | CPS4 |
| ATOM | 2982 | CD1 | | 25 | 0.301 | 33.345 | 28.716 | 1.00 29.02 | CPS4 |
| MOTA | 2983 | CD2 | | 25 | 1.023 | 34.837 | 26.986 | 1.00 29.76 | CPS4 |
| ATOM | 2984 | CE1 | PHE | 25 | 1.576 | 33.380 | 29.286 | 1.00 29.84 | CPS4 |
| MOTA | 2985 | CE2 | PHE | 25 | 2.304 | 34.879 | 27.547 | 1.00 31.14 | CPS4 |
| MOTA | 2986 | CZ | PHE | 25 | 2.579 | 34.146 | 28.699 | 1.00 28.80 | CPS4 |
| MOTA | 2987 | C | PHE | 25 | -0.822 | 31.763 | 25.857 | 1.00 24.98 | CPS4 |
| ATOM | 2988 | 0 | PHE | 25 | 0.244 | 31.385 | 25.364 | 1.00 25.69 | CPS4 |
| ATOM | 2989 | N | ALA | 26 | -1.569 | 30.979 | 26.627 | 1.00 23.55 | CPS4 |
| MOTA | 2990 | CA | ALA | 26 | -1.158 | 29.609 | 26.932 | 1.00 23.50 | CPS4 |
| ATOM | 2991 | CB | ALA | 26 | -2.187 | 28.935 | 27.812 | 1.00 23.29 | CPS4 |
| MOTA | 2992 | C | ALA | 26 | -0.968 | 28.785 | 25.668 | 1.00 23.71 | CPS4 |
| ATOM | 2993 | ō | ALA | 26 | -0.022 | 27.999 | 25.567 | 1.00 22.90 | CPS4 |
| ATOM | 2994 | N | GLU | 27 | -1.887 | 28.951 | 24.719 | 1.00 23.56 | CPS4 |
| ATOM | 2995 | CA | GLU | 27 | -1.837 | 28.211 | 23.460 | 1.00 23.91 | CPS4 |
| | 2996 | | GLU | 27 | -3.114 | 28.471 | 22.645 | 1.00 25.46 | CPS4 |
| ATOM | | CB | | | | | 23.184 | 1.00 28.50 | CPS4 |
| ATOM | 2997 | CG | GLU | 27 | -4.387 | 27.805 | | 1.00 28.30 | CPS4 |
| ATOM | 2998 | CD | GLU | 27 | -4.892 | 28.403 | 24.499 | | CPS4 |
| ATOM | 2999 | | GLU | 27 | -4.603 | 29.589 | 24.774 | 1.00 31.29 | |
| MOTA | 3000 | | GLU | 27 | -5.589 | 27.682 | 25.255 | 1.00 33.07 | CPS4 |
| MOTA | 3001 | C | GLU | 27 | -0.610 | 28.550 | 22.615 | 1.00 23.66 | CPS4 |
| MOTA | 3002 | 0 | GLU | 27 | ~0.152 | 27.734 | 21.822 | 1.00 24.71 | CPS4 |
| ATOM | 3003 | И | ARG | 28 | -0.081 | 29.754 | 22.779 | 1.00 24.04 | CPS4 |
| MOTA | 3004 | CA | ARG | 28 | 1.094 | 30.170 | 22.016 | 1.00 25.19 | CPS4 |
| MOTA | 3005 | CB | ARG | 28 | 1.191 | 31.696 | 22.047 | 1.00 28.07 | CPS4 |
| ATOM | 3006 | CG | ARG | 28 | 1.800 | 32.351 | 20.829 | 1.00 33.41 | CPS4 |
| MOTA | 3007 | CD | ARG | 28 | 0.994 | 33.602 | 20.446 | 1.00 34.25 | CPS4 |
| ATOM | 3008 | NE | ARG | 28 | 0.767 | 34.484 | 21.592 | 1.00 35.45 | CPS4 |
| MOTA | 3009 | CZ | ARG | 28 | -0.389 | 35.097 | 21.853 | 1.00 37.30 | CPS4 |
| ATOM | 3010 | NHl | ARG | 28 | -1.433 | 34.929 | 21.050 | 1.00 35.32 | CPS4 |
| ATOM | 3011 | | ARG | 28 | -0.506 | 35.871 | 22.928 | 1.00 37.39 | CPS4 |
| ATOM | 3012 | С | ARG | 28 | 2.355 | 29.564 | 22.634 | 1.00 24.51 | CPS4 |
| ATOM | 3013 | ō | ARG | 28 | 3.295 | 29.188 | 21.933 | 1.00 23.41 | CPS4 |
| ATOM | 3014 | N | ILE | 29 | 2.348 | 29.459 | 23.956 | 1.00 22.84 | CPS4 |
| ATOM | 3014 | CA | ILE | 29 | 3.498 | 28.959 | 24.707 | 1.00 23.13 | CPS4 |
| | | | | 29 | 3.498 | 29.482 | 26.175 | 1.00 24.30 | CPS4 |
| MOTA | 3016 | CB | ILE | | | 28.961 | | 1.00 24.45 | CPS4 |
| ATOM | 3017 | | ILE | 29 | 4.666 | 31.014 | | 1.00 25.98 | CPS4 |
| ATOM | 3018 | | ILE | 29 | 3.390 | | | 1.00 23.36 | CPS4 |
| ATOM | 3019 | | ILE | 29 | 4.519 | 31.704 | | | CPS4 |
| ATOM | 3020 | C | ILE | 29 | 3.628 | 27.450 | 24.787 | 1.00 22.56 | CF34 |

| ATOM | 3021 | 0 | ILE | 29 | 4.739 | 26.914 | 24.700 | 1.00 22.11 | CPS4 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| ATOM | 3022 | | LEU | 30 | 2.492 | 26.774 | 24.952 | 1.00 20.94 | CPS4 |
| | | | | | | | | | |
| MOTA | 3023 | | LEU | 30 | 2.456 | 25.334 | 25.150 | 1.00 20.47 | CPS4 |
| MOTA | 3024 | CB | LEU | 30 | 1.447 | 25.009 | 26.264 | 1.00 20.33 | CPS4 |
| MOTA | 3025 | CG | LEU | 30 | 1.660 | 25.741 | 27.600 | 1.00 23.00 | CPS4 |
| ATOM | 3026 | CD1 | LEU | 30 | 0.511 | 25.425 | 28.561 | 1.00 23.25 | CPS4 |
| ATOM | 3027 | CD2 | LEU | 30 | 2.999 | 25.331 | 28.199 | 1.00 20.84 | CPS4 |
| ATOM | 3028 | C | LEU | 30 | 2.120 | 24.493 | 23.936 | 1.00 21.35 | CPS4 |
| ATOM | 3029 | 0 | LEU | 30 | 1.279 | 24.870 | 23.127 | 1.00 22.16 | CPS4 |
| MOTA | 3030 | N | THR | 31 | 2.781 | 23.344 | 23.821 | 1.00 21.39 | CPS4 |
| ATOM | 3031 | CA | THR | 31 | 2.505 | 22.428 | 22.727 | 1.00 22.79 | CPS4 |
| | | | | | 3.594 | | | 1.00 22.73 | CPS4 |
| ATOM | 3032 | CB | THR | 31 | | 21.347 | 22.587 | | |
| MOTA | 3033 | | THR | 31 | 3.631 | 20.550 | 23.778 | 1.00 24.29 | CPS4 |
| ATOM | 3034 | CG2 | | 31 | 4.960 | 21.996 | 22.356 | 1.00 24.52 | CPS4 |
| MOTA | 3035 | С | THR | 31 | 1.186 | 21.736 | 23.052 | 1.00 25.13 | CPS4 |
| MOTA | 3036 | 0 | THR | 31 | 0.646 | 21.868 | 24.158 | 1.00 24.76 | CPS4 |
| MOTA | 3037 | N | ARG | 32 | 0.672 | 20.974 | 22.096 | 1.00 27.56 | CPS4 |
| ATOM | 3038 | CA | ARG | 32 | -0.594 | 20.289 | 22.298 | 1.00 30.79 | CPS4 |
| ATOM | 3039 | CB | ARG | 32 | -0.951 | 19.489 | 21.041 | 1.00 33.62 | CPS4 |
| ATOM | 3040 | CG | ARG | 32 | -2,328 | 19.807 | 20.476 | 1.00 38.29 | CPS4 |
| ATOM | 3041 | CD | ARG | 32 | -3.419 | 18.876 | 21.014 | 1.00 42.11 | CPS4 |
| | | NE | ARG | 32 | -4.044 | 19.329 | 22.259 | 1.00 45.08 | CPS4 |
| MOTA | 3042 | | | | | | | 1.00 46.06 | CPS4 |
| ATOM | 3043 | CZ | ARG | 32 | -4.676 | 20.491 | 22.409 | | |
| ATOM | 3044 | NH1 | | 32 | -4.774 | 21.348 | 21.393 | 1.00 45.64 | CPS4 |
| MOTA | 3045 | NH2 | | 32 | -5.224 | 20.792 | 23.577 | 1.00 45.73 | CPS4 |
| MOTA | 3046 | C | ARG | 32 | -0.577 | 19.384 | 23.524 | 1.00 30.10 | CPS4 |
| ATOM | 3047 | 0 | ARG | 32 | -1.527 | 19.388 | 24.310 | 1.00 30.78 | CPS4 |
| ATOM | 3048 | N | SER | 33 | 0.499 | 18.620 | 23.699 | 1.00 30.30 | CPS4 |
| ATOM | 3049 | CA | SER | 33 | 0.615 | 17.722 | 24.850 | 1.00 31.44 | CPS4 |
| MOTA | 3050 | CB | SER | 33 | 1,853 | 16.833 | 24.715 | 1.00 32.43 | CPS4 |
| MOTA | 3051 | OG | SER | 33 | 1.709 | 15.944 | 23.620 | 1.00 37.42 | CPS4 |
| ATOM | 3052 | С | SER | 33 | 0.684 | 18.489 | 26.168 | 1.00 30.59 | CPS4 |
| ATOM | 3053 | Ō | SER | 33 | 0.054 | 18.108 | 27.153 | 1.00 31.00 | CPS4 |
| ATOM | 3054 | N | GLU | 34 | 1.464 | 19.564 | 26.191 | 1.00 28.83 | CPS4 |
| ATOM | 3055 | CA | GLU | 34 | 1.589 | 20.370 | 27.400 | 1.00 27.36 | CPS4 |
| | | | GLU | 34 | 2.621 | 21.487 | 27.192 | 1.00 26.46 | CPS4 |
| ATOM | 3056 | CB | | | | | 27.099 | 1.00 24.49 | CPS4 |
| ATOM | 3057 | CG | GLU | 34 | 4.048 | 20.963 | | | CPS4 |
| MOTA | 3058 | CD | GLU | 34 | 5.074 | 22.029 | 26.712 | 1.00 24.80 | |
| MOTA | 3059 | | GLU | 34 | 6.223 | 21.934 | 27.196 | 1.00 23.27 | CPS4 |
| ATOM | 3060 | OE2 | | 34 | 4.748 | 22.943 | 25.920 | 1.00 23.10 | CPS4 |
| ATOM | 3061 | С | GLU | 34 | 0.232 | 20.962 | 27.757 | 1.00 27.85 | CPS4 |
| ATOM | 3062 | 0 | GLU | 34 | -0.138 | 21.028 | 28.928 | 1.00 27.48 | CPS4 |
| ATOM | 3063 | N | LEU | 35 | -0.513 | 21.392 | 26.742 | 1.00 28.18 | CPS4 |
| ATOM | 3064 | CA | LEU | 35 | -1.840 | 21.960 | 26.968 | 1.00 29.32 | CPS4 |
| ATOM | 3065 | CB | LEU | 35 | -2.428 | 22.478 | 25.657 | 1.00 27.71 | CPS4 |
| ATOM | 3066 | CG | LEU | 35 | -1.986 | 23.882 | 25.261 | 1.00 28.10 | CPS4 |
| ATOM | 3067 | | LEU | 35 | -2.379 | 24.130 | 23.810 | 1.00 28.81 | CPS4 |
| | | | LEU | 35 | -2.629 | 24.928 | 26.202 | 1.00 25.30 | CPS4 |
| ATOM | 3068 | | | | | | 27.572 | 1.00 30.93 | CPS4 |
| ATOM | 3069 | C | LEU | 35 | -2.782 | 20.931 | | 1.00 30.33 | CPS4 |
| ATOM | 3070 | 0 | LEU | 35 | -3.617 | 21.263 | 28.417 | | CPS4 |
| ATOM | 3071 | N | ASP | 36 | -2.659 | 19.681 | 27.135 | 1.00 33.94 | |
| MOTA | 3072 | CA | ASP | 36 | -3.513 | 18.632 | 27.673 | 1.00 35.97 | CPS4 |
| MOTA | 3073 | CB | ASP | 36 | -3.206 | 17.274 | 27.025 | 1.00 37.70 | CPS4 |
| ATOM | 3074 | CG | ASP | 36 | -3.763 | 17.156 | 25.612 | 1.00 39.64 | CPS4 |
| ATOM | 3075 | OD1 | ASP | 36 | -4.838 | 17.727 | 25.332 | 1.00 41.16 | CPS4 |
| ATOM | 3076 | | ASP | 36 | -3.134 | 16.475 | | 1.00 42.22 | CPS4 |
| ATOM | 3077 | C | ASP | 36 | -3.306 | 18.560 | | 1.00 36.01 | CPS4 |
| ATON | 2011 | _ | | -0 | 2.200 | | | | |

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| ATOM | 3078 | 0 | ASP | 36 | -4.269 | 18.440 | 29.933 | 1.00 36.88 | CPS4 |
|------|------|-----|-----|---------------|--------|-------------------|--------|------------|------|
| MOTA | 3079 | N | GLN | 37 | -2.054 | 18.645 | 29.626 | 1.00 35.23 | CPS4 |
| ATOM | 3080 | CA | GLN | 37 | -1.750 | 18.612 | 31.057 | 1.00 34.91 | CPS4 |
| ATOM | 3081 | CB | GLN | 37 | -0.238 | 18.552 | 31.278 | 1.00 36.27 | CPS4 |
| ATOM | 3082 | CG | GLN | 37 | 0.417 | 17.271 | 30.798 | 1.00 40.16 | CPS4 |
| ATOM | 3083 | CD | GLN | 37 | 1.925 | 17.394 | 30.676 | 1.00 41.54 | CPS4 |
| ATOM | 3084 | | GLN | 37 | 2.436 | 18.146 | 29.845 | 1.00 42.68 | CPS4 |
| ATOM | 3085 | | GLN | 37 | 2.647 | 16.656 | 31.509 | 1.00 43.46 | |
| ATOM | 3086 | C | GLN | 37 | -2.302 | | | | CPS4 |
| | | | | | | 19.869 | 31.722 | 1.00 33.96 | CPS4 |
| MOTA | 3087 | 0 | GLN | 37 | -2.985 | 19.810 | 32.743 | 1.00 33.94 | CPS4 |
| ATOM | 3088 | Ŋ | TYR | 38 | -1.990 | 21.009 | 31.120 | 1.00 32.47 | CPS4 |
| MOTA | 3089 | CA | TYR | 38 | -2.422 | 22.315 | 31.601 | 1.00 31.95 | CPS4 |
| ATOM | 3090 | CB | TYR | 38 | -1.938 | 23.378 | 30.617 | 1.00 30.34 | CPS4 |
| ATOM | 3091 | CG | TYR | 38 | -2.442 | 24.776 | 30.869 | 1.00 29.96 | CPS4 |
| MOTA | 3092 | | TYR | 38 | -3.488 | 25.308 | 30.110 | 1.00 30.42 | CPS4 |
| ATOM | 3093 | CEI | | 38 | -3.905 | 26.618 | 30.287 | 1.00 30.73 | CPS4 |
| MOTA | 3094 | CD2 | TYR | 38 | -1.836 | 25.593 | 31.821 | 1.00 28.80 | CPS4 |
| ATOM | 3095 | CE2 | TYR | 38 | -2.248 | 26.906 | 32.005 | 1.00 29.56 | CPS4 |
| ATOM | 3096 | CZ | TYR | 38 | -3.278 | 27.411 | 31.238 | 1.00 31.46 | CPS4 |
| ATOM | 3097 | OH | TYR | 38 | -3.689 | 28.710 | 31.428 | 1.00 32.91 | CPS4 |
| MOTA | 3098 | C | TYR | 38 | -3.936 | 22.438 | 31.803 | 1.00 32.87 | CPS4 |
| MOTA | 3099 | 0 | TYR | 38 | -4.388 | 22.888 | 32.854 | 1.00 31.90 | CPS4 |
| ATOM | 3100 | N | TYR | 39 | -4.716 | 22.040 | 30.801 | 1.00 34.25 | CPS4 |
| MOTA | 3101 | CA | TYR | 39 | -6.167 | 22.151 | 30.905 | 1.00 36.14 | CPS4 |
| MOTA | 3102 | CB | TYR | 39 | -6.842 | 21.687 | 29.605 | 1.00 36.53 | CPS4 |
| ATOM | 3103 | CG | TYR | 39 | -6.618 | 22.577 | 28.390 | 1.00 36.61 | CPS4 |
| ATOM | 3104 | CD1 | TYR | 39 | -6.608 | 23.970 | 28.504 | 1.00 36.59 | CPS4 |
| MOTA | 3105 | CEl | TYR | 39 | -6.471 | 24.791 | 27.378 | 1.00 37.06 | CPS4 |
| MOTA | 3106 | CD2 | TYR | 39 | -6.483 | 22.021 | 27.115 | 1.00 36.55 | CPS4 |
| MOTA | 3107 | CE2 | TYR | 39 | -6.347 | 22.830 | 25.980 | 1.00 37.48 | CPS4 |
| ATOM | 3108 | CZ | TYR | 39 | -6.343 | 24.213 | 26.118 | 1.00 37.69 | CPS4 |
| MOTA | 3109 | OH | TYR | 39 | -6.224 | 25.011 | 24.998 | 1.00 37.54 | CPS4 |
| MOTA | 3110 | C | TYR | 39 | -6.734 | 21.354 | 32.080 | 1.00 37.42 | CPS4 |
| ATOM | 3111 | 0 | TYR | 39 | -7.809 | 21.667 | 32.584 | 1.00 38.66 | CPS4 |
| MOTA | 3112 | N | GLU | 40 | -6.010 | 20.334 | 32.524 | 1.00 39.15 | CPS4 |
| ATOM | 3113 | CA | GLU | 40 | -6.476 | 19.491 | 33.622 | 1.00 41.54 | CPS4 |
| MOTA | 3114 | CB | GLU | 40 | -5.862 | 18.094 | 33.502 | 1.00 43.99 | CPS4 |
| ATOM | 3115 | CG | GLU | 40 | -6.257 | 17.341 | 32.235 | 1.00 48.54 | CPS4 |
| ATOM | 3116 | CD | GLU | 40 | -7.761 | 17.149 | 32.111 | 1.00 50.97 | CPS4 |
| ATOM | 3117 | OEl | GLU | 40 | -8.377 | 16.647 | 33.076 | 1.00 53.41 | CPS4 |
| MOTA | 3118 | OE2 | GLU | 40 | -8.329 | 17.495 | 31.050 | 1.00 52.53 | CPS4 |
| ATOM | 3119 | C | GLU | 40 | -6.181 | 20.035 | 35.009 | 1.00 41.32 | CPS4 |
| MOTA | 3120 | 0 | GLU | 40 | -6.687 | 19.516 | 36.006 | 1.00 41.95 | CPS4 |
| ATOM | 3121 | N | LEU | 41 | -5.374 | 21.085 | 35.075 | 1.00 40.03 | CPS4 |
| ATOM | 3122 | CA | LEU | 41 | -4.988 | 21.666 | 36.353 | 1.00 38.83 | CPS4 |
| MOTA | 3123 | CB | LEU | 41 | -3.589 | 22.283 | 36.230 | 1.00 37.58 | CPS4 |
| ATOM | 3124 | CG | LEU | 41 | -2.457 | 21.303 | 35.908 | 1.00 36.93 | CPS4 |
| ATOM | 3125 | CD1 | LEU | 41 | -1.171 | 22.070 | 35.673 | 1.00 36.17 | CPS4 |
| ATOM | 3126 | CD2 | LEU | 41 | -2.291 | 20.309 | 37.050 | 1.00 36.43 | CPS4 |
| ATOM | 3127 | C | LEU | 41 | -5.939 | 22.709 | 36.916 | 1.00 38.96 | CPS4 |
| ATOM | 3128 | 0 | LEU | 41 | -6.744 | 23.295 | 36.197 | 1.00 38.34 | CPS4 |
| ATOM | 3129 | N | SER | 42 | -5.830 | 22.936 | 38.220 | 1.00 39.70 | CPS4 |
| ATOM | 3130 | CA | SER | 42 | -6.645 | 23.937 | 38.890 | 1.00 41.21 | CPS4 |
| ATOM | 3131 | CB | SER | 42 | -6.456 | 23.849 | 40.408 | 1.00 41.87 | CPS4 |
| ATOM | 3132 | OG | SER | 42 | -5.119 | 24.152 | 40.781 | 1.00 40.52 | CPS4 |
| ATOM | 3133 | C | SER | 42 | -6.182 | 25.305 | 38.399 | 1.00 42.49 | CPS4 |
| ATOM | 3134 | 0 | SER | 42 | -5.134 | 25.424 | 37.766 | 1.00 42.26 | CPS4 |
| | | | | · | • | · - • | _ | | |

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| TI TTO M | 2125 | 3.7 | CTTT | 4.7 | C 0CC | 26 220 | 20 702 | 3 00 40 07 | 0704 |
|----------|------|-----|-------|-----|--------|--------|--------|------------|------|
| MOTA | 3135 | N | GLU | 43 | -6.955 | 26.338 | 38.703 | 1.00 42.87 | CPS4 |
| MOTA | 3136 | CA | GLU | 43 | -6.516 | 27.687 | 38.286 | 1.00 44.09 | CPS4 |
| MOTA | 3137 | CB | GLU | 43 | -7.686 | 28.651 | 38.803 | 1.00 46.92 | CPS4 |
| ATOM | 3138 | CG | GLU | 43 | -7.721 | 30.000 | 38.115 | 1.00 51.91 | CPS4 |
| MOTA | 3139 | CD | GLU | 43 | -6.722 | 30.982 | 38.687 | 1.00 55.38 | CPS4 |
| ATOM | 3140 | OEl | GLU | 43 | -6.747 | 31.203 | 39.920 | 1.00 57.45 | CPS4 |
| ATOM | 3141 | OE2 | GLU | 43 | -5.920 | 31.543 | 37.905 | 1.00 57.72 | CPS4 |
| MOTA | 3142 | c | GLU | 43 | -5.226 | 28.088 | 38.802 | 1.00 43.04 | CPS4 |
| ATOM | 3143 | ō | GLU | 43 | -4.404 | 28.633 | 38.058 | 1.00 42.48 | CPS4 |
| | | | | | | | | 1.00 42.48 | |
| ATOM | 3144 | N | LYS | 44 | -4.965 | 27.805 | 40.074 | | CPS4 |
| MOTA | 3145 | CA | LYS | 44 | -3.684 | 28.136 | 40.690 | 1.00 40.46 | CPS4 |
| MOTA | 3146 | CB | LYS | 44 | -3.758 | 27.910 | 42.201 | 1.00 42.16 | CPS4 |
| MOTA | 3147 | CG | LYS | 44 | -2.528 | 28.378 | 42.960 | 1.00 44.29 | CPS4 |
| MOTA | 3148 | CD | LYS | 44 | -2.684 | 28.137 | 44.457 | 1.00 47.29 | CPS4 |
| ATOM | 3149 | CE | LYS | 44 | -1.439 | 28.574 | 45.218 | 1.00 48.62 | CPS4 |
| MOTA | 3150 | NZ | LYS | 44 | -1.554 | 28.319 | 46.683 | 1.00 50.30 | CPS4 |
| MOTA | 3151 | С | LYS | 44 | -2.537 | 27.311 | 40.107 | 1.00 38.58 | CPS4 |
| ATOM | 3152 | 0 | LYS | 44 | -1.466 | 27.845 | 39.806 | 1.00 37.53 | CPS4 |
| ATOM | 3153 | N | ARG | 4.5 | -2.764 | 26.010 | 39.957 | 1.00 35.62 | CPS4 |
| ATOM | 3154 | CA | ARG | 45 | -1.755 | 25.115 | 39.406 | 1.00 34.29 | CPS4 |
| ATOM | 3155 | CB | ARG | 45 | -2.205 | 23.663 | 39.575 | 1.00 36.05 | CPS4 |
| ATOM | 3156 | CG | ARG | 45 | -2.054 | 23.119 | 41.002 | 1.00 39.56 | CPS4 |
| | | | | | | 22.768 | 41.301 | 1.00 42.27 | CPS4 |
| MOTA | 3157 | CD | ARG | 45 | -0.605 | | | | |
| MOTA | 3158 | NE | ARG | 45 | -0.090 | 21.793 | 40.341 | 1.00 45.82 | CPS4 |
| ATOM | 3159 | CZ | ARG | 45 | 1.003 | 21.973 | 39.600 | 1.00 48.25 | CPS4 |
| ATOM | 3160 | | ARG | 45 | 1.711 | 23.093 | 39.707 | 1.00 47.45 | CPS4 |
| MOTA | 3161 | NH2 | | 45 | 1.381 | 21.037 | 38.733 | 1.00 48.96 | CPS4 |
| ATOM | 3162 | C | ARG | 45 | -1.491 | 25.422 | 37.926 | 1.00 32.63 | CPS4 |
| ATOM | 3163 | 0 | ARG | 45 | -0.383 | 25.215 | 37.425 | 1.00 30.48 | CPS4 |
| MOTA | 3164 | N | LYS | 46 | -2.513 | 25.912 | 37.232 | 1.00 30.94 | CPS4 |
| MOTA | 3165 | CA | LYS | 46 | -2.365 | 26.265 | 35.820 | 1.00 31.41 | CPS4 |
| ATOM | 3166 | CB | LYS | 46 | -3.672 | 26.841 | 35.262 | 1.00 31.76 | CPS4 |
| MOTA | 3167 | CG | LYS | 46 | -4.637 | 25.828 | 34.661 | 1.00 32.98 | CPS4 |
| ATOM | 3168 | CD | LYS | 46 | -5.770 | 26.574 | 33.959 | 1.00 35.55 | CPS4 |
| ATOM | 3169 | CE | LYS | 46 | -6.597 | 25.647 | 33.081 | 1.00 37.38 | CPS4 |
| ATOM | 3170 | NZ | LYS | 46 | -7.283 | 24.614 | 33.895 | 1.00 39.63 | CPS4 |
| ATOM | 3171 | C | LYS | 46 | -1.275 | 27.326 | 35.668 | 1.00 30.10 | CPS4 |
| ATOM | 3172 | 0 | LYS | 46 | -0.365 | 27.197 | 34.843 | 1.00 28.86 | CPS4 |
| | | | ASN | 47 | -1.378 | 28.388 | 36.457 | 1.00 29.05 | CPS4 |
| ATOM | 3173 | N | | | -0.393 | 29.445 | 36.357 | 1.00 29.35 | CPS4 |
| MOTA | 3174 | CA | ASN | 47 | | | | 1.00 23.33 | CPS4 |
| ATOM | 3175 | CB | ASN | 47 | -0.875 | 30.700 | 37.081 | | CPS4 |
| ATOM | 3176 | CG | ASN | 47 | -1.923 | 31.471 | 36.270 | 1.00 36.22 | |
| MOTA | 3177 | | . ASN | 47 | -1.748 | 31.710 | 35.065 | 1.00 37.87 | CPS4 |
| MOTA | 3178 | ND2 | ASN | 47 | -3.008 | 31.869 | 36.928 | 1.00 38.04 | CPS4 |
| MOTA | 3179 | C | ASN | 47 | 0.998 | 29.033 | 36.822 | 1.00 28.34 | CPS4 |
| MOTA | 3180 | 0 | ASN | 47 | 1.987 | 29.533 | 36.291 | 1.00 26.63 | CPS4 |
| MOTA | 3181 | N | GLU | 48 | 1.085 | 28.125 | 37.794 | 1.00 27.39 | CPS4 |
| MOTA | 3182 | CA | GLU | 48 | 2.398 | 27.656 | 38.253 | 1.00 26.57 | CPS4 |
| ATOM | 3183 | CB | GLU | 48 | 2.256 | 26.763 | 39.493 | 1.00 29.29 | CPS4 |
| ATOM | 3184 | CG | GLU | 48 | 1.753 | 27.481 | 40.733 | 1.00 35.14 | CPS4 |
| ATOM | 3185 | CD | GLU | 48 | 1.467 | 26.534 | 41.899 | 1.00 38.18 | CPS4 |
| ATOM | 3186 | | GLU | 48 | 1.054 | 27.029 | 42.970 | 1.00 39.62 | CPS4 |
| | | | GLU | 48 | 1.654 | 25.301 | 41.747 | 1.00 39.49 | CPS4 |
| MOTA | 3187 | | | | | | | 1.00 33.43 | CPS4 |
| ATOM | 3188 | C | GLU | 48 | 3.023 | 26.848 | 37.114 | 1.00 24.53 | CPS4 |
| MOTA | 3189 | 0 | GLU | 48 | 4.198 | 27.004 | 36.786 | | |
| MOTA | 3190 | N | PHE | 49 | 2.215 | 25.984 | | 1.00 22.65 | CPS4 |
| ATOM | 3191 | CA | PHE | 49 | 2.643 | 25.136 | 35.400 | 1.00 22.71 | CPS4 |

| ATOM | 3192 | CB | PHE | 49 | 1.474 | 24.235 | 34.972 | 1.00 23.78 | CPS4 |
|------|------|-----|------------|----------|--------|--------|--------|------------|--------------|
| ATOM | 3193 | CG | PHE | 49 | 1.796 | 23.299 | 33.836 | 1.00 23.79 | CPS4 |
| MOTA | 3194 | CD1 | PHE | 49 | 2.359 | 22.053 | 34.084 | 1.00 25.06 | CPS4 |
| ATOM | 3195 | CD2 | | 49 | 1.525 | 23.660 | 32.522 | 1.00 24.25 | CPS4 |
| ATOM | 3196 | CE1 | | 49 | 2.645 | 21.179 | 33.045 | 1.00 25.26 | CPS4 |
| ATOM | 3197 | | PHE | 49 | 1.812 | 22.786 | 31.464 | 1.00 25.16 | CPS4 |
| ATOM | 3198 | CZ | PHE | 49 | 2.370 | 21.546 | 31.729 | 1.00 26.61 | CPS4 |
| ATOM | 3199 | C | PHE | 49 | 3.089 | 25.980 | 34.201 | 1.00 22.04 | CPS4 |
| ATOM | 3200 | 0 | PHE | 49 | 4.158 | 25.751 | 33.631 | 1.00 21.19 | CPS4 |
| ATOM | 3200 | N | LEU | 50 | 2.260 | 26.945 | 33.818 | 1.00 21.13 | CPS4 |
| MOTA | | | LEU | | 2.564 | 27.807 | | 1.00 21.02 | CPS4 |
| | 3202 | CA | | 50 | | | 32.678 | | |
| ATOM | 3203 | CB | LEU | 50 | 1.386 | 28.749 | 32.389 | 1.00 21.73 | CPS4 |
| ATOM | 3204 | CG | LEU | 50 | 1.487 | 29.682 | 31.172 | 1.00 24.05 | CPS4 |
| MOTA | 3205 | CD1 | | 50 | 1.697 | 28.873 | 29.891 | 1.00 24.04 | CPS4 |
| ATOM | 3206 | CD2 | | 50 | 0.218 | 30.518 | 31.075 | 1.00 23.32 | CPS4 |
| ATOM | 3207 | C | LEU | 50 | 3.832 | 28.624 | 32.922 | 1.00 21.21 | CPS4 |
| ATOM | 3208 | 0 | LEU | 50 | 4.680 | 28.724 | 32.039 | 1.00 20.96 | CPS4 |
| MOTA | 3209 | N | ALA | 51 | 3.960 | 29.207 | 34.114 | 1.00 19.78 | CPS4 |
| ATOM | 3210 | CA | ALA | 51 | 5.150 | 30.005 | 34.432 | 1.00 19.68 | CPS4 |
| ATOM | 3211 | CB | ALA | 51 | 5.017 | 30.616 | 35.830 | 1.00 20.19 | CPS4 |
| MOTA | 3212 | С | ALA | 51 | 6.417 | 29.151 | 34.350 | 1.00 20.59 | CPS4 |
| ATOM | 3213 | 0 | ALA | 51 | 7.453 | 29.598 | 33.830 | 1.00 20.05 | CPS4 |
| ATOM | 3214 | N | GLY | 52 | 6.325 | 27.928 | 34.865 | 1.00 20.38 | CPS4 |
| MOTA | 3215 | CA | GLY | 52 | 7.459 | 27.015 | 34.840 | 1.00 20.83 | CPS4 |
| ATOM | 3216 | С | GLY | 52 | 7.861 | 26.619 | 33.429 | 1.00 20.53 | CPS4 |
| ATOM | 3217 | 0 | GLY | 52 | 9.048 | 26.587 | 33.104 | 1.00 20.29 | CPS4 |
| MOTA | 3218 | N | ARG | 53 | 6.884 | 26.279 | 32.593 | 1.00 21.19 | CPS4 |
| MOTA | 3219 | CA | ARG | 53 | 7.187 | 25.916 | 31.207 | 1.00 21.65 | CPS4 |
| ATOM | 3220 | CB | ARG | 53 | 5.938 | 25.336 | 30.532 | 1.00 23.50 | CPS4 |
| ATOM | 3221 | CG | ARG | 53 | 5.824 | 23.807 | 30.654 | 1.00 26.67 | CPS4 |
| MOTA | 3222 | CD | ARG | 53 | 5.988 | 23.291 | 32.077 | 1.00 31.06 | CPS4 |
| MOTA | 3223 | NE | ARG | 53 | 5.877 | 21.832 | 32.121 | 1.00 35.13 | CPS4 |
| ATOM | 3224 | CZ | ARG | 53 | 6.220 | 21.082 | 33.164 | 1.00 38.06 | CPS4 |
| MOTA | 3225 | NHl | ARG | 53 | 6.702 | 21.649 | 34.267 | 1.00 38.57 | CPS4 |
| ATOM | 3226 | NH2 | ARG | 53 | 6.086 | 19.762 | 33.105 | 1.00 39.34 | CPS4 |
| ATOM | 3227 | С | ARG | 53 | 7.710 | 27.140 | 30.445 | 1.00 20.71 | CPS4 |
| ATOM | 3228 | 0 | ARG | 53 | 8.598 | 27.030 | 29.606 | 1.00 20.01 | CPS4 |
| ATOM | 3229 | N | PHE | 54 | 7.160 | 28.311 | 30.740 | 1.00 20.84 | CPS4 |
| ATOM | 3230 | CA | PHE | 54 | 7.613 | 29.545 | 30.090 | 1.00 19.84 | CPS4 |
| ATOM | 3231 | CB | PHE | 54 | 6.742 | 30.722 | 30.558 | 1.00 19.76 | CPS4 |
| ATOM | 3232 | CG | PHE | 54 | 7.131 | 32.059 | 29.966 | 1.00 22.53 | CPS4 |
| ATOM | 3233 | | PHE | 54 | 7.984 | 32.922 | 30.654 | 1.00 21.19 | CPS4 |
| ATOM | 3234 | | PHE | 54 | 6.638 | 32.457 | 28.728 | 1.00 22.55 | CPS4 |
| ATOM | 3235 | | PHE | 54 | 8.339 | 34.162 | 30.115 | 1.00 22.92 | CPS4 |
| ATOM | 3236 | | PHE | 54 | 6.989 | 33.701 | 28.181 | 1.00 24.30 | CPS4 |
| ATOM | 3237 | CZ | PHE | 54 | 7.846 | 34.553 | 28.883 | 1.00 22.82 | CPS4 |
| MOTA | 3238 | C | PHE | 54 | 9.086 | 29.791 | 30.452 | 1.00 20.51 | CPS4 |
| ATOM | 3239 | 0 | PHE | 54 | 9.912 | 30.084 | 29.583 | 1.00 19.99 | CPS4 |
| | | | | 55 | 9.419 | 29.656 | 31.735 | 1.00 19.95 | CPS4 |
| ATOM | 3240 | N | ALA ALA | 55 55 | 10.798 | 29.874 | 32.179 | 1.00 18.42 | CPS4 |
| ATOM | 3241 | CA | ALA | | | 29.874 | 33.712 | 1.00 17.59 | CPS4 |
| ATOM | 3242 | CB | | 55 | 10.885 | 29.789 | 33.712 | 1.00 17.33 | CPS4 |
| MOTA | 3243 | C | ALA | 55 55 | 11.747 | | | 1.00 18.74 | CPS4 |
| MOTA | 3244 | 0 | ALA | 55 | 12.840 | 29.228 | 31.097 | 1.00 17.67 | CPS4 |
| MOTA | 3245 | N | ALA | 56 | 11.329 | 27.608 | 31.470 | | CPS4 |
| MOTA | 3246 | CA | ALA | 56 | 12.173 | 26.570 | 30.870 | 1.00 17.97 | CPS4 |
| MOTA | 3247 | CB | ALA | 56 | 11.519 | 25.179 | 31.051 | 1.00 16.50 | CPS4 CPS4 |
| MOTA | 3248 | C | ALA | 56 | 12.435 | 26.845 | 29.391 | 1.00 17.61 | CPS4 |

| ATOM | 3249 | 0 | ALA | 56 | 13.555 | 26.672 | 28.898 | 1.00 17.56 | CPS4 |
|------|------|----|-----|----|--------|--------|--------|------------|------|
| ATOM | 3250 | N | LYS | 57 | 11.411 | 27.286 | 28.669 | 1.00 17.23 | CPS4 |
| MOTA | 3251 | | LYS | 57 | 11.603 | 27.555 | 27.249 | 1.00 17.45 | CPS4 |
| MOTA | 3252 | CB | LYS | 57 | 10.243 | 27.657 | 26.535 | 1.00 17.90 | CPS4 |
| ATOM | 3253 | CG | LYS | 57 | 9.470 | 26.320 | 26.585 | 1.00 17.50 | CPS4 |
| ATOM | 3254 | CD | LYS | 57 | 8.243 | 26.286 | 25.673 | 1.00 19.16 | CPS4 |
| ATOM | 3255 | CE | LYS | 57 | 7.453 | 24.998 | 25.915 | 1.00 20.14 | CPS4 |
| ATOM | 3256 | NZ | LYS | 57 | 6.468 | 24.688 | 24.832 | 1.00 18.82 | CPS4 |
| MOTA | 3257 | C | LYS | 57 | 12.450 | 28.800 | 27.033 | 1.00 18.57 | CPS4 |
| MOTA | 3258 | 0 | LYS | 57 | 13.282 | 28.840 | 26.123 | 1.00 18.35 | CPS4 |
| ATOM | 3259 | N | GLU | 58 | 12.254 | 29.815 | 27.863 | 1.00 19.33 | CPS4 |
| ATOM | 3260 | CA | GLU | 58 | 13.057 | 31.018 | 27.733 | 1.00 19.47 | CPS4 |
| ATOM | 3261 | CB | GLU | 58 | 12.581 | 32.104 | 28.698 | 1.00 21.46 | CPS4 |
| ATOM | 3262 | CG | GLU | 58 | 11.276 | 32.786 | 28.308 | 1.00 24.96 | CPS4 |
| ATOM | 3263 | CD | GLU | 58 | 11.375 | 33.576 | 27.003 | 1.00 28.39 | CPS4 |
| ATOM | 3264 | | GLU | 58 | 12.482 | 34.040 | 26.654 | 1.00 30.73 | CPS4 |
| MOTA | 3265 | | GLU | 58 | 10.333 | 33.748 | 26.333 | 1.00 31.57 | CPS4 |
| ATOM | 3266 | C | GLU | 58 | 14.504 | 30.649 | 28.047 | 1.00 19.45 | CPS4 |
| ATOM | 3267 | 0 | GLU | 58 | 15.424 | 31.075 | 27.338 | 1.00 18.48 | CPS4 |
| ATOM | 3268 | N | ALA | 59 | 14.718 | 29.857 | 29.097 | 1.00 17.21 | CPS4 |
| ATOM | 3269 | CA | ALA | 59 | 16.095 | 29.458 | 29.434 | 1.00 16.93 | CPS4 |
| ATOM | 3270 | CB | ALA | 59 | 16.130 | 28.630 | 30.730 | 1.00 16.23 | CPS4 |
| MOTA | 3271 | C | ALA | 59 | 16.704 | 28.663 | 28.288 | 1.00 17.64 | CPS4 |
| MOTA | 3272 | 0 | ALA | 59 | 17.868 | 28.871 | 27.917 | 1.00 18.71 | CPS4 |
| ATOM | 3272 | N | PHE | 60 | 15.925 | 27.752 | 27.708 | 1.00 17.49 | CPS4 |
| ATOM | 3274 | CA | PHE | 60 | 16.438 | 26.973 | 26.590 | 1.00 17.61 | CPS4 |
| ATOM | 3275 | CB | PHE | 60 | 15.404 | 25.953 | 26.093 | 1.00 17.74 | CPS4 |
| ATOM | 3276 | CG | PHE | 60 | 15.860 | 25.203 | 24.869 | 1.00 19.99 | CPS4 |
| ATOM | 3277 | | PHE | 60 | 16.682 | 24.085 | 24.992 | 1.00 21.60 | CPS4 |
| MOTA | 3278 | | PHE | 60 | 15.565 | 25.681 | 23.594 | 1.00 21.01 | CPS4 |
| ATOM | 3279 | | PHE | 60 | 17.214 | 23.453 | 23.863 | 1.00 21.01 | CPS4 |
| MOTA | 3280 | | PHE | 60 | 16.092 | 25.059 | 22.452 | 1.00 20.43 | CPS4 |
| ATOM | 3281 | cz | PHE | 60 | 16.922 | 23.941 | 22.595 | 1.00 22.76 | CPS4 |
| ATOM | 3282 | C | PHE | 60 | 16.817 | 27.894 | 25.423 | 1.00 16.99 | CPS4 |
| ATOM | 3283 | ō | PHE | 60 | 17.853 | 27.701 | 24.792 | 1.00 18.28 | CPS4 |
| ATOM | 3284 | N | SER | 61 | 15.983 | 28.894 | 25.139 | 1.00 17.64 | CPS4 |
| ATOM | 3285 | CA | SER | 61 | 16.263 | 29.801 | 24.026 | 1.00 17.54 | CPS4 |
| MOTA | 3286 | CB | SER | 61 | 15.069 | 30.757 | 23.788 | 1.00 18.97 | CPS4 |
| ATOM | 3287 | OG | SER | 61 | 15.017 | 31.816 | 24.738 | 1.00 20.70 | CPS4 |
| ATOM | 3288 | C | SER | 61 | 17.554 | 30.586 | 24.261 | 1.00 18.58 | CPS4 |
| ATOM | 3289 | ō | SER | 61 | 18.257 | 30.932 | 23.312 | 1.00 19.96 | CPS4 |
| ATOM | 3290 | N | LYS | 62 | 17.873 | 30.856 | 25.520 | 1.00 17.38 | CPS4 |
| ATOM | 3291 | CA | LYS | 62 | 19.095 | 31.579 | 25.855 | 1.00 18.60 | CPS4 |
| ATOM | 3292 | СВ | LYS | 62 | 19.021 | 32.120 | 27.281 | 1.00 19.12 | CPS4 |
| MOTA | 3293 | CG | LYS | 62 | 17.939 | 33.199 | 27.436 | 1.00 24.19 | CPS4 |
| MOTA | 3294 | CD | LYS | 62 | 17.990 | 33.882 | 28.791 | 1.00 27.64 | CPS4 |
| ATOM | 3295 | CE | LYS | 62 | 17.112 | 35.126 | 28.763 | 1.00 31.95 | CPS4 |
| ATOM | 3296 | NZ | LYS | 62 | 17.485 | 36.123 | 29.784 | 1.00 34.09 | CPS4 |
| ATOM | 3297 | С | LYS | 62 | 20.309 | 30.684 | 25.699 | 1.00 18.38 | CPS4 |
| ATOM | 3298 | ō | LYS | 62 | 21.375 | 31.133 | 25.259 | 1.00 19.22 | CPS4 |
| ATOM | 3299 | N | ALA | 63 | 20.156 | 29.418 | 26.070 | 1.00 17.11 | CPS4 |
| ATOM | 3300 | CA | ALA | 63 | 21.248 | 28.460 | 25.934 | 1.00 17.76 | CPS4 |
| MOTA | 3301 | СВ | ALA | 63 | 20.878 | 27.114 | 26.619 | 1.00 16.67 | CPS4 |
| ATOM | 3302 | С | ALA | 63 | 21.497 | | 24.445 | 1.00 18.66 | CPS4 |
| ATOM | 3303 | ō | ALA | 63 | 22.640 | | 24.012 | 1.00 17.98 | CPS4 |
| ATOM | 3304 | N | PHE | 64 | 20.412 | | 23.672 | 1.00 18.77 | CPS4 |
| ATOM | 3305 | CA | PHE | 64 | 20.480 | | 22.220 | 1.00 19.86 | CPS4 |
| | | | | | | | | | |

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| ATOM | 3306 | CB | PHE | 64 | 19.068 | 27.758 | 21.659 | 1.00 21.49 | CPS4 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| MOTA | 3307 | CG | PHE | 64 | 19.049 | 27.258 | 20.239 | 1.00 23.19 | CPS4 |
| MOTA | 3308 | CD1 | PHE | 64 | 19.603 | 26.019 | 19.917 | 1.00 25.84 | CPS4 |
| ATOM | 3309 | CD2 | PHE | 64 | 18.498 | 28.038 | 19.223 | 1.00 24.38 | CPS4 |
| MOTA | 3310 | CEl | PHE | 64 | 19.612 | 25.558 | 18.592 | 1.00 27.01 | CPS4 |
| ATOM | 3311 | CE2 | PHE | 64 | 18.495 | 27.595 | 17.897 | 1.00 25.99 | CPS4 |
| ATOM | 3312 | CZ | PHE | 64 | 19.055 | 26.353 | 17.578 | 1.00 25.96 | CPS4 |
| MOTA | 3313 | C | PHE | 64 | 21.142 | 29.177 | 21.547 | 1.00 21.18 | CPS4 |
| | | 0 | PHE | 64 | 21.687 | 29.057 | 20.446 | 1.00 22.00 | CPS4 |
| ATOM | 3314 | | | | | | | | |
| ATOM | 3315 | И | GLY | 65 | 21.075 | 30.330 | 22.214 | 1.00 20.65 | CPS4 |
| MOTA | 3316 | CA | GLY | 65 | 21.711 | 31.547 | 21.735 | 1.00 21.45 | CPS4 |
| MOTA | 3317 | С | GLY | 65 | 20.914 | 32.487 | 20.848 | 1.00 23.53 | CPS4 |
| MOTA | 3318 | 0 | GLY | 65 | 21.453 | 33.483 | 20.370 | 1.00 24.12 | CPS4 |
| MOTA | 3319 | N | THR | 66 | 19.635 | 32.195 | 20.640 | 1.00 22.34 | CPS4 |
| ATOM | 3320 | CA | THR | 66 | 18.807 | 33.016 | 19.755 | 1.00 23.68 | CPS4 |
| ATOM | 3321 | CB | THR | 66 | 18.176 | 32.144 | 18.667 | 1.00 25.10 | CPS4 |
| MOTA | 3322 | OG1 | THR | 66 | 17.343 | 31.160 | 19.296 | 1.00 25.13 | CPS4 |
| ATOM | 3323 | CG2 | THR | 66 | 19.249 | 31.434 | 17.845 | 1.00 26.27 | CPS4 |
| ATOM | 3324 | С | THR | 66 | 17.646 | 33.737 | 20.424 | 1.00 24.40 | CPS4 |
| ATOM | 3325 | ō | THR | 66 | 17.172 | 34.762 | 19.925 | 1.00 23.79 | CPS4 |
| MOTA | 3326 | N | GLY | 67 | 17.184 | 33.199 | 21.546 | 1.00 23.11 | CPS4 |
| ATOM | 3327 | CA | GLY | 67 | 16.018 | 33.766 | 22.193 | 1.00 22.95 | CPS4 |
| | | | | 67 | 14.822 | 33.246 | 21.391 | 1.00 23.58 | CPS4 |
| ATOM | 3328 | C | GLY | | | | | 1.00 23.38 | CPS4 |
| MOTA | 3329 | 0 | GLY | 67 | 14.997 | 32.581 | 20.369 | 1.00 22.81 | |
| ATOM | 3330 | N | ILE | 68 | 13.610 | 33.540 | 21.848 | | CPS4 |
| ATOM | 3331 | CA | ILE | 68 | 12.401 | 33.107 | 21.150 | 1.00 25.43 | CPS4 |
| MOTA | 3332 | CB | ILE | 68 | 11.194 | 33.083 | 22.110 | 1.00 25.71 | CPS4 |
| MOTA | 3333 | CG2 | | 68 | 9.899 | 32.729 | 21.345 | 1.00 26.85 | CPS4 |
| MOTA | 3334 | CG1 | | 68 | 11.449 | 32.061 | 23.222 | 1.00 24.50 | CPS4 |
| ATOM | 3335 | CD1 | ILE | 68 | 11.495 | 30.626 | 22.739 | 1.00 24.17 | CPS4 |
| MOTA | 3336 | C | ILE | 68 | 12.129 | 34.086 | 20.007 | 1.00 27.56 | CPS4 |
| ATOM | 3337 | 0 | ILE | 68 | 12.150 | 35.300 | 20.203 | 1.00 27.28 | CPS4 |
| ATOM | 3338 | N | GLY | 69 | 11.890 | 33.559 | 18.813 | 1.00 27.53 | CPS4 |
| MOTA | 3339 | CA | GLY | 69 | 11.641 | 34.434 | 17.686 | 1.00 30.15 | CPS4 |
| ATOM | 3340 | C | GLY | 69 | 11.685 | 33.725 | 16.353 | 1.00 30.54 | CPS4 |
| ATOM | 3341 | ō | GLY | 69 | 11.274 | 32.575 | 16.240 | 1.00 30.54 | CPS4 |
| ATOM | 3342 | N | ALA | 70 | 12.197 | 34.416 | 15.342 | 1.00 32.70 | CPS4 |
| ATOM | 3342 | CA | ALA | 70 | 12.272 | 33.860 | 13.998 | 1.00 33.34 | CPS4 |
| | | | | 70 | | 34.886 | 13.043 | 1.00 35.40 | CPS4 |
| MOTA | 3344 | CB | ALA | | 12.896 | 32.551 | 13.043 | 1.00 33.40 | CPS4 |
| MOTA | 3345 | C | ALA | 70 | 13.038 | | | 1.00 33.31 | CPS4 |
| MOTA | 3346 | 0 | ALA | 70 | 12.695 | 31.679 | 13.118 | 1.00 34.32 | CPS4 |
| ATOM | 3347 | N | GLN | 71 | 14.061 | 32.398 | 14.752 | | CPS4 |
| ATOM | 3348 | CA | GLN | 71 | 14.882 | 31.192 | 14.713 | 1.00 30.79 | |
| MOTA | 3349 | CB | GLN | 71 | 16.334 | 31.545 | 15.039 | 1.00 33.45 | CPS4 |
| MOTA | 3350 | CG | GLN | 71 | 16.936 | 32.597 | 14.127 | 1.00 37.57 | CPS4 |
| MOTA | 3351 | CD | GLN | 71 | 18.391 | 32.873 | 14.451 | 1.00 38.92 | CPS4 |
| MOTA | 3352 | OE1 | GLN | 71 | 19.258 | 32.016 | 14.257 | 1.00 40.93 | CPS4 |
| MOTA | 3353 | NE2 | GLN | 71 | 18.665 | 34.069 | 14.961 | 1.00 40.14 | CPS4 |
| ATOM | 3354 | С | GLN | 71 | 14.443 | 30.066 | 15.636 | 1.00 28.73 | CPS4 |
| ATOM | 3355 | 0 | GLN | 71 | 14.851 | 28.923 | 15.454 | 1.00 28.34 | CPS4 |
| ATOM | 3356 | N | LEU | 72 | 13.626 | 30.384 | 16.633 | 1.00 26.49 | CPS4 |
| ATOM | 3357 | CA | LEU | 72 | 13.182 | 29.369 | | 1.00 24.09 | CPS4 |
| | | CB | LEU | 72 | 14.224 | 29.221 | 18.690 | 1.00 24.17 | CPS4 |
| MOTA | 3358 | | | | | 28.183 | | 1.00 23.09 | CPS4 |
| ATOM | 3359 | CG | LEU | 72 | 13.988 | | | 1.00 23.74 | CPS4 |
| MOTA | 3360 | | LEU | 72 | 14.211 | 26.785 | | 1.00 25.05 | CPS4 |
| ATOM | 3361 | | LEU | 72 | 14,948 | 28.457 | | | CPS4 |
| MOTA | 3362 | С | LEU | 72 | 11.847 | 29.777 | 18.169 | 1.00 23.32 | CF34 |
| | | | | | | | | | |

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| MOTA | 3363 | 0 | LEU | 72 | 11.699 | 30.876 | 18.688 | 1.00 24.09 | CPS4 |
|------|------|-----|-----|------------|--------|--------|--------|------------|------|
| MOTA | 3364 | N | SER | 73 | 10.880 | 28.877 | 18.084 | 1.00 22.99 | CPS4 |
| ATOM | 3365 | CA | SER | 73 | 9.542 | 29.112 | 18.601 | 1.00 23.16 | CPS4 |
| ATOM | 3366 | CB | SER | 73 | 8.527 | 28.653 | 17.555 | 1.00 23.80 | CPS4 |
| ATOM | 3367 | OG | SER | 73 | 7.227 | 28.611 | 18.093 | 1.00 29.93 | CPS4 |
| ATOM | 3368 | C | SER | 73 | 9.297 | 28.339 | 19.896 | 1.00 22.31 | CPS4 |
| ATOM | 3369 | ō | SER | 73 | 9.976 | 27.353 | 20.175 | 1.00 21.09 | |
| ATOM | 3370 | N | PHE | 74 | 8.334 | 28.803 | | | CPS4 |
| | | | | | | | 20.692 | 1.00 22.33 | CPS4 |
| MOTA | 3371 | CA | PHE | 74 | 7.962 | 28.093 | 21.914 | 1.00 21.01 | CPS4 |
| ATOM | 3372 | CB | PHE | 74 | 6.802 | 28.801 | 22.625 | 1.00 21.02 | CPS4 |
| MOTA | 3373 | CG | PHE | 74 | 7.201 | 30.032 | 23.386 | 1.00 23.04 | CPS4 |
| MOTA | 3374 | CD1 | | 74 | 8.018 | 29.937 | 24.508 | 1.00 23.64 | CPS4 |
| MOTA | 3375 | CD2 | PHE | 74 | 6.726 | 31.285 | 23.003 | 1.00 22.57 | CPS4 |
| ATOM | 3376 | CEl | PHE | 74 | 8.355 | 31.074 | 25.246 | 1.00 25.06 | CPS4 |
| ATOM | 3377 | CE2 | PHE | 74 | 7.057 | 32.423 | 23.728 | 1.00 25.56 | CPS4 |
| ATOM | 3378 | CZ | PHE | 74 | 7.872 | 32.318 | 24.854 | 1.00 24.29 | CPS4 |
| ATOM | 3379 | Ċ | PHE | 74 | 7.470 | 26.714 | 21.479 | 1.00 21.66 | CPS4 |
| ATOM | 3380 | ō | PHE | 74 | 7.567 | 25.744 | 22.224 | 1.00 20.92 | CPS4 |
| ATOM | 3381 | И | GLN | 75 | 6.928 | 26.635 | 20.266 | 1.00 20.29 | CPS4 |
| ATOM | 3382 | CA | GLN | 75 | 6.402 | 25.372 | 19.760 | 1.00 20.29 | CPS4 |
| | | | | | | | | | |
| MOTA | 3383 | CB | GLN | 75 | 5.442 | 25.637 | 18.595 | 1.00 22.50 | CPS4 |
| MOTA | 3384 | CG | GLN | 75 | 4.216 | 26.457 | 18.996 | 1.00 22.28 | CPS4 |
| MOTA | 3385 | ÇD | GLN | 75 | 3.364 | 25.763 | 20.048 | 1.00 22.84 | CPS4 |
| MOTA | 3386 | | GLN | 75 | 2.914 | 26.384 | 21.020 | 1.00 25.78 | CPS4 |
| ATOM | 3387 | NE2 | GLN | 75 | 3.133 | 24.471 | 19.858 | 1.00 21.79 | CPS4 |
| ATOM | 3388 | C | GLN | 75 | 7.482 | 24.374 | 19.334 | 1.00 21.34 | CPS4 |
| ATOM | 3389 | 0 | GLN | 75 | 7.179 | 23.209 | 19.072 | 1.00 22.34 | CPS4 |
| ATOM | 3390 | N | ASP | 76 | 8.732 | 24.835 | 19.277 | 1.00 20.43 | CPS4 |
| ATOM | 3391 | CA | ASP | 76 | 9.872 | 23.989 | 18.903 | 1.00 20.89 | CPS4 |
| ATOM | 3392 | CB | ASP | 76 | 11.006 | 24.827 | 18.294 | 1.00 22.04 | CPS4 |
| ATOM | 3393 | CG | ASP | 76 | 10.672 | 25.375 | 16.922 | 1.00 25.59 | CPS4 |
| MOTA | 3394 | | ASP | 76 | 10.016 | 24.658 | 16.149 | 1.00 28.36 | CPS4 |
| MOTA | 3395 | | ASP | 76 | 11.094 | 26.513 | 16.614 | 1.00 25.63 | CPS4 |
| MOTA | 3396 | C | ASP | 76 | 10.442 | 23.292 | 20.132 | 1.00 20.74 | CPS4 |
| | | | | 76 76 | | | 20.132 | 1.00 20.74 | CPS4 |
| MOTA | 3397 | 0 | ASP | | 11.380 | 22.499 | | | |
| MOTA | 3398 | N | ILE | 7 7 | 9.869 | 23.586 | 21.291 | 1.00 19.74 | CPS4 |
| MOTA | 3399 | CA | ILE | 77 | 10.353 | 23.033 | 22.551 | 1.00 19.49 | CPS4 |
| ATOM | 3400 | CB | ILE | 7 7 | 10.944 | 24.160 | 23.433 | 1.00 18.31 | CPS4 |
| ATOM | 3401 | CG2 | ILE | 77 | 11.700 | 23.554 | 24.627 | 1.00 19.88 | CPS4 |
| ATOM | 3402 | CG1 | | 77 | 11.856 | 25.056 | 22.584 | 1.00 19.12 | CPS4 |
| MOTA | 3403 | CD1 | ILE | 77 | 12.172 | 26.401 | 23.232 | 1.00 18.75 | CPS4 |
| ATOM | 3404 | С | ILE | 77 | 9.249 | 22.387 | 23.356 | 1.00 20.14 | CPS4 |
| MOTA | 3405 | 0 | ILE | 77 | 8.162 | 22.932 | 23.474 | 1.00 21.52 | CPS4 |
| MOTA | 3406 | N | GLU | 78 | 9.530 | 21.233 | 23.942 | 1.00 20.14 | CPS4 |
| MOTA | 3407 | CA | GLU | 78 | 8.520 | 20.590 | 24.760 | 1.00 21.03 | CPS4 |
| ATOM | 3408 | CB | GLU | 78 | 7.814 | 19.483 | | 1.00 22.66 | CPS4 |
| ATOM | 3409 | CG | GLU | 78 | 6.792 | 18.707 | | 1.00 23.61 | CPS4 |
| ATOM | 3410 | CD | GLU | 78 | 5.914 | 17.815 | | 1.00 26.69 | CPS4 |
| | | | | 78 | 5.039 | | 23.195 | 1.00 26.76 | CPS4 |
| ATOM | 3411 | | GLU | | | 18.352 | | 1.00 23.70 | CPS4 |
| ATOM | 3412 | | GLU | 78 | 6.105 | 16.581 | 23.922 | | |
| ATOM | 3413 | C | GLU | 78 | 9.153 | 20.025 | 26.014 | 1.00 20.86 | CPS4 |
| MOTA | 3414 | 0 | GLU | 78 | 10.219 | 19.411 | 25.953 | 1.00 20.47 | CPS4 |
| ATOM | 3415 | N | ILE | 79 | 8.519 | 20.273 | 27.158 | 1.00 20.68 | CPS4 |
| MOTA | 3416 | CA | ILE | 79 | 9.019 | 19.744 | 28.420 | 1.00 21.74 | CPS4 |
| ATOM | 3417 | CB | ILE | 79 | 8.845 | 20.756 | 29.598 | 1.00 24.16 | CPS4 |
| ATOM | 3418 | CG2 | ILE | 79 | 9.053 | 20.044 | | 1.00 23.26 | CPS4 |
| ATOM | 3419 | | ILE | 79 | 9.868 | 21.891 | | | CPS4 |
| | | | | | | | | | |

| ATOM | 3420 | CD1 | TILE | 79 | 9.772 | 22.726 | 28.227 | 1.00 28.49 | CPS4 |
|------|--------------|-----|----------------|----|--------|--------|--------|------------|------|
| ATOM | 3421 | C | ILE | 79 | 8.234 | 18.478 | 28.748 | 1.00 22.41 | CPS4 |
| | | | | | | | | | |
| MOTA | 3422 | 0 | ILE | 79 | 7.001 | 18.462 | 28.685 | 1.00 22.59 | CPS4 |
| MOTA | 3423 | N | ARG | 80 | 8.958 | 17.417 | 29.075 | 1.00 22.76 | CPS4 |
| MOTA | 3424 | CA | ARG | 80 | 8.349 | 16.151 | 29.451 | 1.00 24.99 | CPS4 |
| MOTA | 3425 | CB | ARG | 80 | 8.684 | 15.081 | 28.419 | 1.00 25.33 | CPS4 |
| ATOM | 3426 | CG | ARG | 80 | 8.181 | 15.426 | 27.038 | 1.00 28.31 | CPS4 |
| ATOM | 3427 | CD | ARG | 80 | 8.496 | 14.332 | 26.049 | 1.00 31.70 | CPS4 |
| MOTA | 3428 | NE | ARG | 80 | 7.736 | 14.538 | 24.828 | 1.00 33.61 | CPS4 |
| MOTA | 3429 | CZ | ARG | 80 | 7.701 | 13.677 | 23.820 | 1.00 35.93 | CPS4 |
| MOTA | 3430 | NH1 | | 80 | 8.390 | 12.545 | 23.893 | 1.00 34.86 | CPS4 |
| | | | | | | | | | CPS4 |
| MOTA | 3431 | | ARG | 80 | 6.974 | 13.952 | 22.743 | 1.00 35.80 | |
| ATOM | 3432 | C | ARG | 80 | 8.938 | 15.777 | 30.802 | 1.00 26.08 | CPS4 |
| ATOM | 3433 | 0 | ARG | 80 | 9.892 | 16.412 | 31.257 | 1.00 22.69 | CPS4 |
| ATOM | 3434 | N | LYS | 81 | 8.372 | 14.760 | 31.448 | 1.00 27.41 | CPS4 |
| MOTA | 3435 | CA | LYS | 81 | 8.877 | 14.334 | 32.750 | 1.00 29.89 | CPS4 |
| MOTA | 3436 | CB | LYS | 81 | 7.866 | 14.652 | 33.858 | 1.00 31.74 | CPS4 |
| ATOM | 3437 | CG | LYS | 81 | 7.741 | 16.134 | 34.201 | 1.00 36.20 | CPS4 |
| ATOM | 3438 | CD | LYS | 81 | 6.836 | 16.335 | 35.421 | 1.00 39.03 | CPS4 |
| ATOM | 3439 | CE | LYS | 81 | 6.576 | 17.813 | 35.724 | 1.00 41.06 | CPS4 |
| ATOM | 3440 | NZ | LYS | 81 | 7.812 | 18.590 | 36.021 | 1.00 41.14 | CPS4 |
| | | | | 81 | 9.157 | 12.844 | 32.742 | 1.00 31.20 | CPS4 |
| ATOM | 3441 | C | LYS | | | | | | CPS4 |
| MOTA | 3442 | 0 | LYS | 81 | 8.378 | 12.069 | 32.185 | 1.00 30.64 | |
| MOTA | 3443 | N | ASP | 82 | 10.270 | 12.432 | 33.341 | 1.00 30.63 | CPS4 |
| MOTA | 3444 | CA | ASP | 82 | 10.567 | 11.010 | 33.374 | 1.00 31.88 | CPS4 |
| ATOM | 3445 | CB | ASP | 82 | 12.073 | 10.746 | 33.491 | 1.00 30.04 | CPS4 |
| ATOM | 3446 | CG | ASP | 82 | 12.670 | 11.248 | 34.788 | 1.00 30.81 | CPS4 |
| ATOM | 3447 | OD1 | ASP | 82 | 11.938 | 11.421 | 35.789 | 1.00 31.13 | CPS4 |
| ATOM | 3448 | QD2 | ASP | 82 | 13.899 | 11.447 | 34.805 | 1.00 31.19 | CPS4 |
| MOTA | 3449 | C | ASP | 82 | 9.820 | 10.351 | 34.523 | 1.00 32.86 | CPS4 |
| MOTA | 3450 | 0 | ASP | 82 | 9.037 | 10.997 | 35.221 | 1.00 32.72 | CPS4 |
| ATOM | 3451 | N | GLN | 83 | 10.063 | 9.059 | 34.710 | 1.00 35.26 | CPS4 |
| ATOM | 3452 | CA | GLN | 83 | 9.404 | 8.292 | 35.755 | 1.00 37.75 | CPS4 |
| | | | GLN | 83 | 9.861 | 6.827 | 35.684 | 1.00 40.68 | CPS4 |
| ATOM | 3453 | CB | | | | | 35.407 | 1.00 45.63 | CPS4 |
| MOTA | 3454 | CG | GLN | 83 | 11.357 | 6.615 | | 1.00 48.44 | CPS4 |
| ATOM | 3455 | CD | GLN | 83 | 11.805 | 7.096 | 34.020 | | |
| ATOM | 3 456 | | GLN | 83 | 11.016 | 7.130 | 33.068 | 1.00 49.61 | CPS4 |
| MOTA | 3457 | NE2 | GLN | 83 | 13.086 | 7.447 | 33.901 | 1.00 50.02 | CPS4 |
| MOTA | 3458 | C | GLN | 83 | 9.607 | 8.854 | 37.160 | 1.00 38.09 | CPS4 |
| ATOM | 3459 | 0 | GLN | 83 | 8.748 | 8.688 | 38.026 | 1.00 38.46 | CPS4 |
| ATOM | 3460 | N | ASN | 84 | 10.733 | 9.528 | 37.386 | 1.00 37.38 | CPS4 |
| ATOM | 3461 | CA | ASN | 84 | 11.012 | 10.119 | 38.692 | 1.00 36.22 | CPS4 |
| MOTA | 3462 | CB | ASN | 84 | 12.520 | 10.213 | 38.931 | 1.00 37.16 | CPS4 |
| MOTA | 3463 | CG | ASN | 84 | 13.170 | 8.858 | 39.110 | 1.00 37.93 | CPS4 |
| | 3464 | | ASN | 84 | 12.631 | 7.984 | 39.787 | 1.00 39.18 | CPS4 |
| ATOM | | | | | 14.343 | 8.682 | 38.518 | 1.00 39.57 | CPS4 |
| MOTA | 3465 | | ASN | 84 | | | | 1.00 36.01 | CPS4 |
| MOTA | 3466 | c | ASN | 84 | 10.404 | 11.512 | 38.834 | 1.00 37.22 | CPS4 |
| MOTA | 3 467 | 0 | ASN | 84 | 10.470 | 12.118 | 39.903 | | |
| MOTA | 3468 | N | \mathtt{GLY} | 85 | 9.817 | 12.027 | 37.759 | 1.00 34.03 | CPS4 |
| ATOM | 346 9 | CA | GLY | 85 | 9.226 | 13.352 | 37.824 | 1.00 31.62 | CPS4 |
| MOTA | 3470 | C | GLY | 85 | 10.203 | 14.446 | 37.408 | 1.00 29.19 | CPS4 |
| MOTA | 3471 | 0 | GLY | 85 | 9.904 | 15.632 | 37.517 | 1.00 28.96 | CPS4 |
| MOTA | 3472 | N | LYS | 86 | 11.377 | 14.048 | 36.938 | 1.00 26.53 | CPS4 |
| ATOM | 3473 | CA | LYS | 86 | 12.394 | 15.009 | 36.507 | 1.00 25.85 | CPS4 |
| ATOM | 3474 | CB | LYS | 86 | 13.775 | 14.336 | 36.511 | 1.00 26.12 | CPS4 |
| | | CG | LYS | 86 | 14.913 | 15.136 | 35.853 | 1.00 24.62 | CPS4 |
| ATOM | 3475 | | | | | 16.357 | | 1.00 22.52 | CPS4 |
| MOTA | 3476 | CD | LYS | 86 | 15.358 | 10.32/ | 30.070 | 1.00 22.32 | |

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| TO COM | 2477 | CE | T 37C | 0.0 | 16 260 | 77 700 | 25 000 | | ~~~. |
|--------|------|-----|-------|-----|--------|--------|--------|------------|------|
| MOTA | 3477 | | LYS | 86 | 16.368 | 17.189 | 35.880 | 1.00 23.49 | CPS4 |
| ATOM | 3478 | ΝZ | LYS | 86 | 17.044 | 18.252 | 36.687 | 1.00 21.98 | CPS4 |
| ATOM | 3479 | C | LYS | 86 | 12.069 | 15.527 | 35.105 | 1.00 25.27 | CPS4 |
| ATOM | 3480 | 0 | LYS | 86 | 11.868 | 14.746 | 34.175 | 1.00 23.72 | CPS4 |
| ATOM | 3481 | N | PRO | 87 | 11.987 | 16.859 | 34.936 | 1.00 24.18 | CPS4 |
| ATOM | | | PRO | 87 | | | | | |
| | 3482 | CD | | | 12.068 | 17.970 | 35.906 | 1.00 24.38 | CPS4 |
| MOTA | 3483 | CA | PRO | 87 | 11.682 | 17.351 | 33.589 | 1.00 23.07 | CPS4 |
| MOTA | 3484 | CB | PRO | 87 | 11.343 | 18.825 | 33.822 | 1.00 24.68 | CPS4 |
| MOTA | 3485 | CG | PRO | 87 | 12.229 | 19.189 | 34.995 | 1.00 24.14 | CPS4 |
| MOTA | 3486 | С | PRO | 87 | 12.869 | 17.202 | 32.658 | 1.00 22.51 | CPS4 |
| ATOM | 3487 | 0 | PRO | 87 | 14.028 | 17.182 | 33.098 | 1.00 21.21 | CPS4 |
| ATOM | 3488 | N | TYR | 88 | 12.576 | 17.094 | 31.366 | 1.00 21.14 | CPS4 |
| | | | | | | | | | |
| ATOM | 3489 | CA | TYR | 88 | 13.617 | 17.009 | 30.363 | 1.00 21.50 | CPS4 |
| MOTA | 3490 | CB | TYR | 88 | 14.069 | 15.563 | 30.132 | 1.00 23.25 | CPS4 |
| MOTA | 3491 | CG | TYR | 88 | 13.032 | 14.648 | 29.546 | 1.00 24.04 | CPS4 |
| ATOM | 3492 | CD1 | TYR | 88 | 12.953 | 14.449 | 28.165 | 1.00 26.52 | CPS4 |
| MOTA | 3493 | CE1 | TYR | 88 | 12.033 | 13.554 | 27.622 | 1.00 27.83 | CPS4 |
| MOTA | 3494 | CD2 | TYR | 88 | 12.164 | 13.941 | 30.369 | 1.00 25.98 | CPS4 |
| MOTA | 3495 | CE2 | TYR | 88 | 11.241 | 13.048 | 29.840 | 1.00 27.07 | CPS4 |
| ATOM | 3496 | CZ | TYR | 88 | 11.185 | 12.857 | 28.467 | 1.00 28.72 | CPS4 |
| | | | | | | | | | |
| MOTA | 3497 | OH | TYR | 88 | 10.295 | 11.941 | 27.945 | 1.00 31.78 | CPS4 |
| MOTA | 3498 | C | TYR | 88 | 13.049 | 17.631 | 29.105 | 1.00 20.69 | CPS4 |
| MOTA | 3499 | 0 | TYR | 88 | 11.839 | 17.679 | 28.915 | 1.00 20.95 | CPS4 |
| MOTA | 3500 | N | ILE | 89 | 13.930 | 18.130 | 28.257 | 1.00 21.21 | CPS4 |
| ATOM | 3501 | CA | ILE | 89 | 13.501 | 18.805 | 27.042 | 1.00 21.24 | CPS4 |
| ATOM | 3502 | CB | ILE | 89 | 14.275 | 20.141 | 26.878 | 1.00 20.12 | CPS4 |
| ATOM | 3503 | CG2 | ILE | 89 | 14.157 | 20.667 | 25.423 | 1.00 21.03 | CPS4 |
| ATOM | 3504 | CG1 | | 89 | 13.757 | 21.164 | 27.900 | 1.00 20.90 | CPS4 |
| | | | | | 14.595 | 22.440 | 28.000 | 1.00 21.80 | CPS4 |
| MOTA | 3505 | CD1 | | 89 | | | | | |
| MOTA | 3506 | С | ILE | 89 | 13.698 | 18.011 | 25.767 | 1.00 22.30 | CPS4 |
| MOTA | 3507 | 0 | ILE | 89 | 14.685 | 17.290 | 25.625 | 1.00 22.10 | CPS4 |
| MOTA | 3508 | N | ILE | 90 | 12.729 | 18.126 | 24.862 | 1.00 22.64 | CPS4 |
| MOTA | 3509 | CA | ILE | 90 | 12.871 | 17.544 | 23.538 | 1.00 23.23 | CPS4 |
| MOTA | 3510 | CB | ILE | 90 | 11.850 | 16.413 | 23.228 | 1.00 25.32 | CPS4 |
| ATOM | 3511 | CG2 | ILE | 90 | 11.987 | 15.303 | 24.259 | 1.00 25.34 | CPS4 |
| ATOM | 3512 | CG1 | | 90 | 10.424 | 16.946 | 23.187 | 1.00 27.66 | CPS4 |
| ATOM | 3513 | CD1 | | 90 | 9.462 | 16.003 | 22.454 | 1.00 29.92 | CPS4 |
| | | | | 90 | 12.609 | | 22.654 | 1.00 23.52 | CPS4 |
| ATOM | 3514 | C | ILE | | | 18.760 | | | |
| ATOM | 3515 | 0 | ILE | 90 | 11.780 | 19.610 | 22.988 | 1.00 23.18 | CPS4 |
| MOTA | 3516 | N | CYS | 91 | 13.341 | 18.892 | 21.558 | 1.00 22.32 | CPS4 |
| ATOM | 3517 | CA | CYS | 91 | 13.118 | 20.042 | 20.692 | 1.00 24.32 | CPS4 |
| ATOM | 3518 | CB | CYS | 91 | 14.023 | 21.209 | 21.096 | 1.00 22.65 | CPS4 |
| MOTA | 3519 | SG | CYS | 91 | 15.776 | 20.862 | 20.976 | 1.00 28.76 | CPS4 |
| ATOM | 3520 | С | CYS | 91 | 13.367 | 19.670 | 19.244 | 1.00 24.59 | CPS4 |
| ATOM | 3521 | 0 | CYS | 91 | 13.834 | 18.575 | 18.947 | 1.00 26.28 | CPS4 |
| ATOM | 3522 | N | THR | 92 | 13.064 | 20.591 | 18.344 | 1.00 25.08 | CPS4 |
| | | | | | | 20.331 | 16.920 | 1.00 25.91 | CPS4 |
| MOTA | 3523 | CA | THR | 92 | 13.234 | | | | CPS4 |
| ATOM | 3524 | CB | THR | 92 | 12.266 | 21.187 | 16.102 | 1.00 26.21 | |
| ATOM | 3525 | OG1 | THR | 92 | 12.577 | 22.562 | 16.329 | 1.00 25.10 | CPS4 |
| ATOM | 3526 | CG2 | THR | 92 | 10.828 | 20.933 | 16.526 | 1.00 25.78 | CPS4 |
| ATOM | 3527 | C | THR | 92 | 14.633 | 20.629 | 16.417 | 1.00 26.72 | CPS4 |
| ATOM | 3528 | Ö | THR | 92 | 14.938 | 20.371 | 15.255 | 1.00 27.72 | CPS4 |
| ATOM | 3529 | N | LYS | 93 | 15.480 | 21.163 | 17.291 | 1.00 26.75 | CPS4 |
| ATOM | 3530 | CA | LYS | 93 | 16.830 | 21.589 | 16.927 | 1.00 28.49 | CPS4 |
| | | | | | | | 17.583 | 1.00 30.97 | CPS4 |
| MOTA | 3531 | CB | LYS | 93 | 17.109 | 22.946 | | 1.00 36.76 | CPS4 |
| MOTA | 3532 | CG | LYS | 93 | 16.792 | 24.162 | 16.729 | | |
| ATOM | 3533 | CD | LYS | 93 | 15.450 | 24.100 | 16.039 | 1.00 38.80 | CPS4 |
| | | | | | | | | | |

| ATOM | 3534 | CE | LYS | 93 | 15.212 | 25.376 | 15.229 | 1.00 40.84 | CPS4 |
|------|--------------|-----|-----|------------|--------|--------|--------|------------|------|
| MOTA | 3535 | NZ | LYS | 93 | 14.048 | 25.250 | 14.312 | 1.00 43.58 | CPS4 |
| MOTA | 3536 | С | LYS | 93 | 18.005 | 20.676 | 17.234 | 1.00 27.51 | CPS4 |
| ATOM | 3537 | 0 | LYS | 93 | 19.005 | 20.676 | 16.509 | 1.00 27.46 | CPS4 |
| MOTA | 3538 | N | LEU | 94 | 17.910 | 19.911 | 18.307 | 1.00 26.01 | CPS4 |
| ATOM | 3539 | CA | LEU | 94 | 19.020 | 19.058 | 18.676 | 1.00 25.30 | CPS4 |
| MOTA | 3540 | CB | LEU | 94 | 20.055 | 19.904 | 19.408 | 1.00 27.33 | CPS4 |
| | | | | | | | | | |
| ATOM | 3541 | CG | LEU | 94 | 19.418 | 20.843 | 20.433 | 1.00 28.62 | CPS4 |
| MOTA | 3542 | CD1 | | 94 | 19.228 | 20.074 | 21.712 | 1.00 30.37 | CPS4 |
| MOTA | 3543 | CD2 | | 94 | 20.292 | 22.060 | 20.673 | 1.00 30.20 | CPS4 |
| MOTA | 3544 | C | LEU | 94 | 18.556 | 17.889 | 19.524 | 1.00 25.14 | CPS4 |
| MOTA | 3545 | 0 | LEU | 94 | 17.414 | 17.854 | 19.974 | 1.00 24.61 | CPS4 |
| MOTA | 3546 | N | SER | 95 | 19.460 | 16.944 | 19.755 | 1.00 24.28 | CPS4 |
| ATOM | 3547 | CA | SER | 95 | 19.153 | 15.731 | 20.499 | 1.00 26.04 | CPS4 |
| MOTA | 3548 | CB | SER | 95 | 20.323 | 14.756 | 20.355 | 1.00 27.48 | CPS4 |
| ATOM | 3549 | OG | SER | 95 | 20.100 | 13.586 | 21.116 | 1.00 33.27 | CPS4 |
| MOTA | 3550 | C | SER | 95 | 18.825 | 15.908 | 21.982 | 1.00 25.21 | CPS4 |
| MOTA | 3551 | 0 | SER | 95 | 19.445 | 16.714 | 22.672 | 1.00 26.64 | CPS4 |
| ATOM | 3552 | N | PRO | 96 | 17.840 | 15.150 | 22.485 | 1.00 25.96 | CPS4 |
| ATOM | 3553 | | PRO | 96 | 16.943 | 14.229 | 21.760 | 1.00 25.56 | CPS4 |
| | | CD | | | | | | 1.00 25.36 | CPS4 |
| ATOM | 3554 | CA | PRO | 96 | 17.461 | 15.245 | 23.900 | | |
| ATOM | 3555 | CB | PRO | 96 | 16.385 | 14.165 | 24.045 | 1.00 26.57 | CPS4 |
| MOTA | 3556 | CG | PRO | 96 | 15.745 | 14.149 | 22.679 | 1.00 27.21 | CPS4 |
| ATOM | 3557 | C | PRO | 96 | 18.677 | 14.961 | 24.787 | 1.00 26.31 | CPS4 |
| MOTA | 3558 | 0 | PRO | 96 | 18.835 | 15.561 | 25.856 | 1.00 24.59 | CPS4 |
| MOTA | 3559 | N | ALA | 97 | 19.541 | 14.056 | 24.323 | 1.00 27.53 | CPS4 |
| ATOM | 3560 | CA | ALA | 97 | 20.739 | 13.678 | 25.074 | 1.00 29.07 | CPS4 |
| MOTA | 3561 | CB | ALA | 97 | 21.480 | 12.589 | 24.286 | 1.00 34.39 | CPS4 |
| ATOM | 3562 | С | ALA | 97 | 21.690 | 14.853 | 25.314 | 1.00 27.61 | CPS4 |
| MOTA | 3563 | 0 | ALA | 97 | 22.492 | 14.827 | 26.251 | 1.00 26.14 | CPS4 |
| ATOM | 3564 | N | ALA | 98 | 21.599 | 15.885 | 24.483 | 1.00 24.18 | CPS4 |
| ATOM | 3565 | CA | ALA | 98 | 22.486 | 17.034 | 24.617 | 1.00 23.38 | CPS4 |
| MOTA | 3565 | CB | ALA | 98 | 22.804 | 17.600 | 23.238 | 1.00 25.54 | CPS4 |
| ATOM | 3567 | C | ALA | 98 | 21.943 | 18.150 | 25.500 | 1.00 23.06 | CPS4 |
| | | | ALA | 98 | 22.634 | 19.140 | 25.730 | 1.00 23.28 | CPS4 |
| MOTA | 3568 | 0 | | | | | | 1.00 23.28 | CPS4 |
| MOTA | 3569 | N | VAL | 99 | 20.720 | 17.993 | 25.999 | | CPS4 |
| ATOM | 3570 | CA | VAL | 99 | 20.109 | 19.048 | 26.796 | 1.00 20.54 | |
| MOTA | 3571 | CB | VAL | 9 9 | 18.806 | 19.548 | 26.146 | 1.00 21.70 | CPS4 |
| ATOM | 3572 | | VAL | 99 | 18.317 | 20.837 | 26.820 | 1.00 20.11 | CPS4 |
| ATOM | 35 73 | | VAL | 99 | 19.026 | 19.777 | 24.692 | 1.00 25.15 | CPS4 |
| MOTA | 3574 | C | VAL | 99 | 19.781 | 18.622 | 28.206 | 1.00 20.45 | CPS4 |
| ATOM | 3575 | 0 | VAL | 99 | 19.399 | 17.477 | 28.450 | 1.00 20.26 | CPS4 |
| MOTA | 3576 | N | HIS | 100 | 19.924 | 19.572 | 29.123 | 1.00 19.96 | CPS4 |
| ATOM | 3577 | CA | HIS | 100 | 19.634 | 19.349 | 30.531 | 1.00 19.64 | CPS4 |
| ATOM | 3578 | CB | HIS | 100 | 20.935 | 19.210 | 31.318 | 1.00 20.91 | CPS4 |
| ATOM | 3579 | CG | HIS | 100 | 21.844 | 18.154 | 30.773 | 1.00 24.67 | CPS4 |
| ATOM | 3580 | | HIS | 100 | 22.842 | 18.227 | 29.862 | 1.00 26.77 | CPS4 |
| ATOM | 3581 | | HIS | 100 | 21.715 | 16.820 | 31.096 | 1.00 26.53 | CPS4 |
| | | | HIS | 100 | 22.593 | 16.115 | 30.403 | 1.00 26.82 | CPS4 |
| ATOM | 3582 | | | | 23.288 | 16.113 | 29.646 | 1.00 28.13 | CPS4 |
| ATOM | 3583 | | HIS | 100 | | | | 1.00 18.58 | CPS4 |
| MOTA | 3584 | C | HIS | 100 | 18.864 | 20.561 | 31.020 | | CPS4 |
| ATOM | 3585 | 0 | HIS | 100 | 19.141 | 21.683 | 30.602 | 1.00 18.37 | |
| MOTA | 3586 | N | VAL | 101 | 17.907 | 20.336 | 31.911 | 1.00 18.87 | CPS4 |
| ATOM | 358 7 | CA | VAL | 101 | 17.103 | 21.434 | 32.431 | 1.00 17.84 | CPS4 |
| ATOM | 3588 | CB | VAL | 101 | 15.800 | 21.590 | 31.608 | 1.00 16.78 | CPS4 |
| ATOM | 3589 | CG1 | VAL | 101 | 14.930 | 20.345 | 31.770 | 1.00 18.44 | CPS4 |
| ATOM | 3590 | CG2 | VAL | 101 | 15.029 | 22.840 | 32.049 | 1.00 18.77 | CPS4 |
| | | | | | | | | | |

| ATOM | 3591 | С | VAL | 101 | 16.723 | 21.199 | 33.879 | 1.00 18.74 | CPS4 |
|------|------|-----|-----|-----|--------|--------|--------|------------|------|
| ATOM | 3592 | 0 | VAL | 101 | 16.711 | 20.069 | 34.350 | 1.00 17.29 | CPS4 |
| ATOM | 3593 | N | SER | 102 | 16.441 | 22.287 | 34.590 | 1.00 18.62 | CPS4 |
| ATOM | 3594 | CA | SER | 102 | 15.980 | 22.193 | 35.963 | 1.00 18.53 | CPS4 |
| ATOM | 3595 | CB | SER | 102 | 17.117 | 22.333 | 36.970 | 1.00 19.00 | CPS4 |
| ATOM | 3596 | OG | SER | 102 | 16.596 | 22.169 | 38.289 | 1.00 19.73 | CPS4 |
| MOTA | 3597 | C | SER | 102 | 15.004 | 23.348 | 36.139 | 1.00 19.67 | CPS4 |
| MOTA | 3598 | 0 | SER | 102 | 15.250 | 24.446 | 35.638 | 1.00 18.04 | CPS4 |
| MOTA | 3599 | N | ILE | 103 | 13.901 | 23.092 | 36.841 | 1.00 19.50 | CPS4 |
| ATOM | 3600 | CA | ILE | 103 | 12.886 | 24.105 | 37.082 | 1.00 19.92 | CPS4 |
| ATOM | 3601 | CB | ILE | 103 | 11.552 | 23.731 | 36.386 | 1.00 22.07 | CPS4 |
| ATOM | 3602 | CG2 | | 103 | 10.527 | 24.867 | 36.551 | 1.00 23.01 | CPS4 |
| ATOM | 3603 | CG1 | | 103 | 11.804 | 23.454 | 34.905 | 1.00 21.39 | CPS4 |
| ATOM | 3604 | CD1 | | 103 | 10.570 | 22.958 | 34.144 | 1.00 21.32 | CPS4 |
| ATOM | 3605 | C | ILE | 103 | 12.642 | 24.173 | 38.590 | 1.00 20.11 | CPS4 |
| ATOM | 3606 | Ō | ILE | 103 | 12.633 | 23.137 | 39.277 | 1.00 20.14 | CPS4 |
| ATOM | 3607 | N | THR | 104 | 12.462 | 25.386 | 39.098 | 1.00 18.69 | CPS4 |
| ATOM | 3608 | CA | THR | 104 | 12.205 | 25.588 | 40.517 | 1.00 21.54 | CPS4 |
| MOTA | 3609 | CB | THR | 104 | 13.492 | 26.019 | 41.274 | 1.00 23.15 | CPS4 |
| ATOM | 3610 | OG1 | THR | 104 | 13.245 | 26.008 | 42.686 | 1.00 23.24 | CPS4 |
| ATOM | 3611 | CG2 | THR | 104 | 13.927 | 27.418 | 40.856 | 1.00 22.71 | CPS4 |
| ATOM | 3612 | C | THR | 104 | 11.113 | 26.639 | 40.698 | 1.00 21.91 | CPS4 |
| ATOM | 3613 | ō | THR | 104 | 10.790 | 27.376 | 39.772 | 1.00 19.56 | CPS4 |
| ATOM | 3614 | N | HIS | 105 | 10.542 | 26.701 | 41.899 | 1.00 22.60 | CPS4 |
| ATOM | 3615 | CA | HIS | 105 | 9.465 | 27.639 | 42.189 | 1.00 24.01 | CPS4 |
| ATOM | 3616 | CB | HIS | 105 | 8.110 | 26.927 | 42.112 | 1.00 26.53 | CPS4 |
| ATOM | 3617 | CG | HIS | 105 | 7.721 | 26.457 | 40.746 | 1.00 30.77 | CPS4 |
| ATOM | 3618 | | HIS | 105 | 7.892 | 25.262 | 40.130 | 1.00 32.51 | CPS4 |
| ATOM | 3619 | | HIS | 105 | 6.995 | 27.237 | 39.871 | 1.00 32.62 | CPS4 |
| ATOM | 3620 | | HIS | 105 | 6.731 | 26.543 | 38.778 | 1.00 32.63 | CPS4 |
| ATOM | 3621 | | HIS | 105 | 7.264 | 25.341 | 38.909 | 1.00 33.46 | CPS4 |
| MOTA | 3622 | C | HIS | 105 | 9.558 | 28.179 | 43.613 | 1.00 24.17 | CPS4 |
| ATOM | 3623 | ō | HIS | 105 | 10.135 | 27.537 | 44.491 | 1.00 22.69 | CPS4 |
| ATOM | 3624 | N | THR | 106 | 8.992 | 29.366 | 43.816 | 1.00 24.57 | CPS4 |
| ATOM | 3625 | CA | THR | 106 | 8.856 | 29.967 | 45.147 | 1.00 24.52 | CPS4 |
| ATOM | 3626 | CB | THR | 106 | 9.756 | 31.195 | 45.408 | 1.00 24.79 | CPS4 |
| ATOM | 3627 | OG1 | | 106 | 9.327 | 32.299 | 44.602 | 1.00 23.92 | CPS4 |
| ATOM | 3628 | CG2 | THR | 106 | 11.210 | 30.858 | 45.127 | 1.00 24.13 | CPS4 |
| ATOM | 3629 | C | THR | 106 | 7.415 | 30.444 | 45.065 | 1.00 26.14 | CPS4 |
| ATOM | 3630 | ō | THR | 106 | 6.756 | 30.249 | 44.034 | 1.00 26.11 | CPS4 |
| ATOM | 3631 | N | LYS | 107 | 6.917 | 31.072 | 46.123 | 1.00 26.83 | CPS4 |
| ATOM | 3632 | CA | LYS | 107 | 5.539 | 31.546 | 46.115 | 1.00 27.90 | CPS4 |
| ATOM | 3633 | CB | LYS | 107 | 5.200 | 32.186 | 47.464 | 1.00 30.86 | CPS4 |
| MOTA | 3634 | CG | LYS | 107 | 3.756 | 32.658 | 47.573 | 1.00 34.83 | CPS4 |
| MOTA | 3635 | CD | LYS | 107 | 3.490 | 33.278 | 48.940 | 1.00 39.94 | CPS4 |
| ATOM | 3636 | CE | LYS | 107 | 2.024 | 33.649 | 49.117 | 1.00 42.44 | CPS4 |
| ATOM | 3637 | NZ | LYS | 107 | 1.755 | 34.215 | 50.479 | 1.00 45.42 | CPS4 |
| ATOM | 3638 | C | LYS | 107 | 5.250 | 32.541 | 44.994 | 1.00 26.50 | CPS4 |
| ATOM | 3639 | ō | LYS | 107 | 4.169 | 32.511 | 44.402 | 1.00 27.10 | CPS4 |
| ATOM | 3640 | N | GLU | 108 | 6.222 | 33.396 | 44.684 | 1.00 24.12 | CPS4 |
| ATOM | 3641 | CA | GLU | 108 | 6.050 | 34.436 | 43.672 | 1.00 23.55 | CPS4 |
| ATOM | 3642 | CB | GLU | 108 | 6.476 | 35.783 | 44.256 | 1.00 27.75 | CPS4 |
| ATOM | 3643 | CG | GLU | 108 | 5.755 | 36.152 | 45.530 | 1.00 34.21 | CPS4 |
| MOTA | 3644 | CD | GLU | 108 | 4.301 | 36.440 | 45.297 | 1.00 39.02 | CPS4 |
| MOTA | 3645 | | GLU | 108 | 3.639 | 35.645 | 44.593 | 1.00 43.65 | CPS4 |
| MOTA | 3646 | | GLU | 108 | 3.813 | 37.463 | 45.823 | 1.00 44.70 | CPS4 |
| ATOM | 3647 | C | GLU | 108 | 6.794 | 34.267 | 42.352 | 1.00 23.22 | CPS4 |
| AION | 204/ | _ | GHO | 100 | 0.134 | J7.40/ | 76.334 | 1.00 20.24 | |

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| ATOM | 3648 | 0 | GLU | 108 | 6.553 | 35.023 | 41.400 | 1.00 22.15 | CPS4 |
|------|--------------|-----|-------|-----|--------|--------|--------|--------------------------|--------------|
| ATOM | 3649 | N | TYR | 109 | 7.711 | 33.308 | 42.293 | 1.00 21.80 | CPS4 |
| ATOM | 3650 | CA | TYR | 109 | 8.509 | 33.129 | 41.077 | 1.00 22.23 | CPS4 |
| ATOM | 3651 | CB | TYR | 109 | 9.940 | 33.626 | 41.317 | 1.00 22.18 | CPS4 |
| MOTA | 3652 | CG | TYR | 109 | 10.035 | 35.082 | 41.674 | 1.00 22.99 | CPS4 |
| MOTA | 3653 | CD1 | | 109 | 9.984 | 36.062 | 40.688 | 1.00 22.71 | CPS4 |
| MOTA | 3654 | CEl | TYR | 109 | 10.017 | 37.418 | 41.018 | 1.00 25.19 | CPS4 |
| ATOM | 3655 | CD2 | TYR | 109 | 10.127 | 35.485 | 43.008 | 1.00 25.01 | CPS4 |
| ATOM | 3656 | CE2 | TYR | 109 | 10.158 | 36.833 | 43.350 | 1.00 26.56 | CPS4 |
| ATOM | 3657 | CZ | TYR | 109 | 10.101 | 37.793 | 42.349 | 1.00 26.58 | CPS4 |
| MOTA | 3658 | OH | TYR | 109 | 10.114 | 39.128 | 42.677 | 1.00 29.10 | CPS4 |
| MOTA | 3659 | С | TYR | 109 | 8.625 | 31.713 | 40.569 | 1.00 20.65 | CPS4 |
| MOTA | 3660 | 0 | TYR | 109 | 8.402 | 30.757 | 41.297 | 1.00 20.79 | CPS4 |
| ATOM | 3661 | N | ALA | 110 | 8.989 | 31.609 | 39.294 | 1.00 21.05 | CPS4 |
| ATOM | 3662 | CA | ALA | 110 | 9.280 | 30.334 | 38.654 | 1.00 19.88 | CPS4 |
| ATOM | 3663 | CB | ALA | 110 | 8.267 | 29.999 | 37.567 | 1.00 21.21 | CPS4 |
| ATOM | 3664 | C | ALA | 110 | 10.638 | 30.617 | 38.028 | 1.00 19.33 | CPS4 |
| MOTA | 3665 | 0 | ALA | 110 | 10.887 | 31.730 | 37.568 | 1.00 20.58 | CPS4 |
| MOTA | 3666 | И | ALA | 111 | 11.525 | 29.626 | 38.008 | 1.00 18.54 | CPS4 |
| ATOM | 3667 | CA | ALA | 111 | 12.842 | 29.834 | 37.423 | 1.00 17.54 | CPS4 |
| ATOM | 3668 | CB | ALA | 111 | 13.840 | 30.291 | 38.498 | 1.00 17.07 | CPS4 |
| ATOM | 3669 | С | ALA | 111 | 13.314 | 28.540 | 36.786 | 1.00 16.63 | CPS4 |
| MOTA | 3670 | 0 | ALA | 111 | 12.873 | 27.454 | 37.160 | 1.00 17.51 | CPS4 |
| MOTA | 3671 | N | ALA | 112 | 14.218 | 28.654 | 35.826 | 1.00 17.15 | CPS4 |
| MOTA | 3672 | CA | ALA | 112 | 14.721 | 27.471 | 35.161 | 1.00 16.51 | CPS4 |
| ATOM | 3673 | CB | ALA | 112 | 13.771 | 27.054 | 34.046 | 1.00 17.29 | CPS4 |
| ATOM | 3674 | C | ALA | 112 | 16.092 | 27.742 | 34.583 | 1.00 16.61 | CPS4 |
| MOTA | 3675 | 0 | ALA | 112 | 16.476 | 28.887 | 34.363 | 1.00 15.97 | CPS4 |
| MOTA | 3676 | N | GLN | 113 | 16.842 | 26.677 | 34.356 | 1.00 17.66 | CPS4 |
| MOTA | 367 7 | CA | GLN | 113 | 18.148 | 26.829 | 33.754 | 1.00 17.26 | CPS4 |
| MOTA | 3678 | CB | GLN | 113 | 19.257 | 26.820 | 34.811 | 1.00 19.62 | CPS4 |
| ATOM | 3679 | CG | GLN | 113 | 19.419 | 25.510 | 35.538 | 1.00 23.20 | CPS4 |
| MOTA | 3680 | CD | GLN | 113 | 20.569 | 25.522 | 36.537 | 1.00 26.68 | CPS4 |
| MOTA | 3681 | | GLN | 113 | 20.942 | 24.480 | 37.077 | 1.00 29.56 | CPS4 |
| MOTA | 3682 | NE2 | | 113 | 21.121 | 26.697 | 36.798 | 1.00 29.78 | CPS4 |
| MOTA | 3683 | С | GLN | 113 | 18.314 | 25.678 | 32.789 | 1.00 17.26 | CPS4 |
| MOTA | 3684 | 0 | GLN | 113 | 17.741 | 24.609 | 32.975 | 1.00 16.60 | CPS4 |
| ATOM | 3685 | N | VAL | 114 | 19.093 | 25.910 | 31.746 | 1.00 16.61 | CPS4 |
| MOTA | 3686 | CA | VAL | 114 | 19.329 | 24.880 | 30.744 | 1.00 17.56 | CPS4 |
| MOTA | 3687 | CB | VAL | 114 | 18.523 | 25.161 | 29.436 | 1.00 17.29 | CPS4 |
| ATOM | 3688 | | VAL | 114 | 19.016 | 24.268 | 28.275 | 1.00 18.95 | CPS4 |
| ATOM | 3689 | | VAL | 114 | 17.058 | 24.895 | 29.671 | 1.00 19.12 | CPS4 |
| MOTA | 3690 | С | VAL | 114 | 20.795 | 24.886 | 30.386 | 1.00 17.66 | CPS4 |
| ATOM | 3691 | 0 | LAV | 114 | 21.454 | 25.938 | 30.404 | 1.00 17.69 | CPS4 CPS4 |
| ATOM | 3692 | N | VAL | 115 | 21.309 | 23.696 | 30.104 | 1.00 18.00 | CPS4 |
| ATOM | 3693 | CA | VAL | 115 | 22.673 | 23.566 | 29.629 | 1.00 18.27 1.00 19.25 | CPS4 |
| ATOM | 3694 | CB | VAL | 115 | 23.611 | 22.872 | 30.635 | 1.00 19.23 | CPS4 |
| MOTA | 3695 | | VAL | 115 | 24.962 | 22.560 | 29.939 | | CPS4 |
| MOTA | 3696 | | VAL | 115 | 23.845 | 23.762 | 31.841 | 1.00 17.55 1.00 19.07 | CPS4 |
| ATOM | 3697 | C | VAL | 115 | 22.597 | 22.696 | 28.378 | 1.00 19.07 | CPS4 |
| ATOM | 3698 | 0 | VAL | 115 | 21.987 | 21.626 | 28.394 | | CPS4 |
| ATOM | 3699 | N | ILE | 116 | 23.197 | 23.170 | 27.293 | 1.00 18.54 | CPS4 |
| ATOM | 3700 | CA | ILE | 116 | 23.236 | 22.407 | 26.053 | 1.00 21.10 1.00 21.01 | CPS4 |
| ATOM | 3701 | CB | ILE | 116 | 22.762 | 23.239 | 24.850 | 1.00 21.01 | CPS4 |
| ATOM | 3702 | | ILE | 116 | 22.921 | 22.420 | 23.563 | | CPS4 |
| MOTA | 3703 | | . ILE | 116 | 21.298 | 23.652 | 25.046 | | CPS4 |
| MOTA | 3704 | CD1 | . ILE | 116 | 20.775 | 24.599 | 23.943 | 1.00 10.08 | CF34 |

| ATOM | 3705 | С | ILE | 116 | 24.692 | 22.029 | 25.851 | 1.00 22.03 | CPS4 |
|------|------|-----|-----|-----|--------|--------|----------------|------------|------|
| ATOM | 3706 | 0 | ILE | 116 | 25.570 | 22.884 | 25.856 | 1.00 21.24 | CPS4 |
| MOTA | 3707 | N | GLU | 117 | 24.951 | 20.736 | 25.702 | 1.00 25.15 | CPS4 |
| ATOM | 3708 | CA | GLU | 117 | 26.317 | 20.266 | 25.509 | 1.00 28.51 | |
| | | CB | GLU | 117 | 26.469 | | | | CPS4 |
| ATOM | 3709 | | | | | 18.835 | 26.012 | 1.00 28.70 | CPS4 |
| ATOM | 3710 | CG | GLU | 117 | 26.237 | 18.661 | 27.490 | 1.00 33.10 | CPS4 |
| ATOM | 3711 | CD | GLU | 117 | 26.513 | 17,240 | 27.929 | 1.00 34.43 | CPS4 |
| MOTA | 3712 | OE1 | GLU | 117 | 27.702 | 16.908 | 28.114 | 1.00 36.09 | CPS4 |
| MOTA | 3713 | OE2 | GLU | 117 | 25.545 | 16.458 | 28.070 | 1.00 35.59 | CPS4 |
| MOTA | 3714 | С | GLU | 117 | 26.677 | 20.279 | 24.041 | 1.00 30.50 | CPS4 |
| ATOM | 3715 | 0 | GLU | 117 | 25.815 | 20.420 | 23.186 | 1.00 29.91 | CPS4 |
| MOTA | 3716 | N | ARG | 118 | 27.960 | 20.137 | 23.747 | 1.00 34.16 | CPS4 |
| ATOM | 3717 | CA | ARG | 118 | 28.371 | 20.085 | 22.355 | 1.00 38.48 | CPS4 |
| ATOM | 3718 | СВ | ARG | 118 | 29.800 | 20.597 | 22.182 | 1.00 41.53 | CPS4 |
| ATOM | 3719 | CG | ARG | 118 | 29.971 | 22.069 | 22.549 | 1.00 45.64 | CPS4 |
| ATOM | 3720 | CD | ARG | 118 | 30.881 | 22.808 | 21.567 | 1.00 47.97 | CPS4 |
| | | | ARG | | | | | | CPS4 |
| ATOM | 3721 | NE | | 118 | 30.154 | 23.472 | 20.477 | 1.00 50.66 | |
| ATOM | 3722 | CZ | ARG | 118 | 29.372 | 22.860 | 19.585 | 1.00 50.73 | CPS4 |
| ATOM | 3723 | NH1 | | 118 | 29.188 | 21.550 | 19.633 | 1.00 52.65 | CPS4 |
| ATOM | 3724 | NH2 | | 118 | 28.786 | 23.560 | 18.622 | 1.00 51.12 | CPS4 |
| ATOM | 3725 | C | ARG | 118 | 28.285 | 18.615 | 21.984 | 1.00 40.15 | CPS4 |
| MOTA | 3726 | OT1 | | 118 | 27.421 | 18.274 | 21.156 | 1.00 41.62 | CPS4 |
| MOTA | 3727 | OT2 | ARG | 118 | 29.063 | 17.816 | 22.555 | 1.00 41.20 | CPS4 |
| ATOM | 3728 | C | GLY | 1 | 28.742 | 14.952 | 31.117 | 1.00 33.66 | CPS5 |
| ATOM | 3729 | 0 | GLY | 1 | 29.119 | 14.581 | 32.234 | 1.00 34.07 | CPS5 |
| ATOM | 3730 | N | GLY | 1 | 30.561 | 13.536 | 30.129 | 1.00 37.12 | CPS5 |
| ATOM | 3731 | CA | GLY | 1 | 29.506 | 14.565 | 29.858 | 1.00 34.50 | CPS5 |
| ATOM | 3732 | N | ILE | 2 | 27.654 | 15.692 | 30.948 | 1.00 31.08 | CPS5 |
| MOTA | 3733 | CA | ILE | 2 | 26.856 | 16.110 | 32.095 | 1.00 28.11 | CPS5 |
| ATOM | 3734 | CB | ILE | 2 | 26.178 | 17.462 | 31.826 | 1.00 27.63 | CPS5 |
| ATOM | 3735 | | ILE | 2 | 25.128 | 17.747 | 32.899 | 1.00 24.45 | CPS5 |
| | 3736 | | ILE | 2 | 27.244 | 18.559 | 31.785 | 1.00 28.90 | CPS5 |
| MOTA | | CD1 | | 2 | 26.695 | 19.935 | 31.484 | 1.00 20.30 | CPS5 |
| ATOM | 3737 | | | | | | | | CPS5 |
| ATOM | 3738 | C | ILE | 2 | 25.797 | 15.083 | 32.441 | 1.00 27.43 | |
| MOTA | 3739 | 0 | ILE | 2 | 25.067 | 14.611 | 31.567 | 1.00 27.84 | CPS5 |
| ATOM | 3740 | N | TYR | 3 | 25.719 | 14.735 | 33.723 | 1.00 27.08 | CPS5 |
| MOTA | 3741 | CA | TYR | 3 | 24.737 | 13.768 | 34.198 | 1.00 27.10 | CPS5 |
| ATOM | 3742 | CB | TYR | 3 | 25.220 | 13.087 | 35.476 | 1.00 30.18 | CPS5 |
| MOTA | 3743 | CG | TYR | 3 | 24.212 | 12.108 | 36.033 | 1.00 34.88 | CPS5 |
| MOTA | 3744 | CD1 | TYR | 3 | 24.012 | 10.862 | 35.428 | 1.00 36.41 | CPS5 |
| MOTA | 3745 | CEl | TYR | 3 | 23.063 | 9.963 | 35.920 | 1.00 38.43 | CPS5 |
| MOTA | 3746 | CD2 | TYR | 3 | 23.435 | 12.433 | 37.146 | 1.00 36.11 | CPS5 |
| ATOM | 3747 | CE2 | TYR | 3 | 22.484 | 11.542 | 37.646 | 1.00 38.38 | CPS5 |
| ATOM | 3748 | CZ | TYR | 3 | 22.305 | 10.309 | 37.029 | 1.00 39.52 | CPS5 |
| ATOM | 3749 | OH | TYR | 3 | 21.378 | 9.418 | 37.530 | 1.00 42.62 | CPS5 |
| ATOM | 3750 | C | TYR | 3 | 23.418 | 14.475 | 34.485 | 1.00 26.49 | CPS5 |
| MOTA | 3751 | ō | TYR | 3 | 22.340 | 13.985 | 34.130 | 1.00 24.87 | CPS5 |
| MOTA | 3752 | И | GLY | 4 | 23.499 | 15.624 | 35.153 | 1.00 24.12 | CPS5 |
| | | | | | | | 35.449 | 1.00 22.31 | CPS5 |
| ATOM | 3753 | CA | GLY | 4 | 22.284 | 16.355 | | | CPS5 |
| MOTA | 3754 | C | GLY | 4 | 22.562 | 17.715 | 36.047 | 1.00 20.04 | |
| ATOM | 3755 | 0 | GLY | 4 | 23.667 | 17.966 | 36.509 | 1.00 20.64 | CPS5 |
| ATOM | 3756 | N | ILE | 5 | 21.572 | 18.602 | 36.011 | 1.00 19.86 | CPS5 |
| ATOM | 3757 | CA | ILE | 5 | 21.730 | 19.932 | 36.592 | 1.00 18.90 | CPS5 |
| MOTA | 3758 | CB | ILE | 5 | 21.865 | 21.055 | 3 5.523 | 1.00 18.93 | CPS5 |
| MOTA | 3759 | CG2 | ILE | 5 | 22.936 | 20.676 | 34.510 | 1.00 18.22 | CPS5 |
| ATOM | 3760 | CG1 | ILE | 5 | 20.521 | 21.321 | 34.835 | 1.00 19.13 | CPS5 |
| ATOM | 3761 | CD1 | ILE | 5 | 20.582 | 22.454 | 33.780 | 1.00 18.31 | CPS5 |
| | | | | | | | | | |

| MOTA | 3762 | С | ILE | 5 | 20.532 | 20,234 | 37.471 | 1.00 18.47 | CPS5 |
|------|------|-----|-----|----|--------|--------|--------|--------------------------|------|
| ATOM | 3763 | 0 | ILE | 5 | 19.456 | 19.655 | 37.309 | 1.00 17.95 | CPS5 |
| ATOM | 3764 | N | GLY | 6 | 20.727 | 21.149 | 38.410 | 1.00 18.51 | CPS5 |
| ATOM | 3765 | CA | GLY | 6 | 19.654 | 21.489 | 39.318 | 1.00 18.44 | CPS5 |
| ATOM | 3766 | Ç | GLY | 6 | 19.741 | 22.925 | 39.766 | 1.00 18.43 | CPS5 |
| ATOM | 3767 | 0 | GLY | 6 | 20.829 | 23.461 | 39.972 | 1.00 18.58 | CPS5 |
| ATOM | 3768 | N | LEU | 7 | 18.572 | 23.530 | 39.916 | 1.00 17.51 | CPS5 |
| ATOM | 3769 | CA | LEU | 7 | 18.429 | 24.910 | 40.337 | 1.00 18.75 | CPS5 |
| ATOM | 3770 | CB | LEU | 7 | 17.977 | 25.769 | 39.146 | 1.00 20.12 | CPS5 |
| ATOM | 3771 | CG | LEU | 7 | 17.715 | 27,246 | 39.457 | 1.00 20.05 | CPS5 |
| ATOM | 3772 | CD1 | LEU | 7 | 19.056 | 27.945 | 39.706 | 1.00 18.90 | CPS5 |
| ATOM | 3773 | | LEU | 7 | 16.967 | 27.907 | 38.298 | 1.00 19.78 | CPS5 |
| ATOM | 3774 | С | LEU | 7 | 17.366 | 24.991 | 41.428 | 1.00 19.75 | CPS5 |
| MOTA | 3775 | 0 | LEU | 7 | 16.329 | 24.330 | 41.353 | 1.00 18.94 | CPS5 |
| ATOM | 3776 | N | ASP | 8 | 17.626 | 25.797 | 42.450 | 1.00 18.42 | CPS5 |
| MOTA | 3777 | CA | ASP | 8 | 16.644 | 25.985 | 43.491 | 1.00 20.59 | CPS5 |
| ATOM | 3778 | CB | ASP | 8 | 16.823 | 24.969 | 44.625 | 1.00 22.60 | CPS5 |
| ATOM | 3779 | CG | ASP | 8 | 15.838 | 25.199 | 45.764 | 1.00 25.07 | CPS5 |
| ATOM | 3780 | | ASP | 8 | 16.142 | 26.008 | 46.666 | 1.00 26.32 | CPS5 |
| ATOM | 3781 | | ASP | 8 | 14.749 | 24.597 | 45.742 | 1.00 26.96 | CPS5 |
| ATOM | 3782 | C | ASP | 8 | 16.700 | 27.391 | 44.066 | 1.00 19.95 | CPS5 |
| ATOM | 3783 | 0 | ASP | 8 | 17.768 | 27.957 | 44.243 | 1.00 21.00 | CPS5 |
| ATOM | 3784 | N | ILE | 9 | 15.533 | 27.966 | 44.309 | 1.00 19.58 | CPS5 |
| ATOM | 3785 | CA | ILE | 9 | 15.456 | 29.275 | 44.949 | 1.00 19.88 | CPS5 |
| ATOM | 3786 | CB | ILE | 9 | 14.814 | 30.352 | 44.055 | 1.00 19.88 | CPS5 |
| ATOM | 3787 | | ILE | 9 | 14.757 | 31.674 | 44.820 | 1.00 19.92 | CPS5 |
| ATOM | 3788 | CG1 | | 9 | 15.640 | 30.524 | 42.776 | 1.00 13.32 | CPS5 |
| ATOM | 3789 | | ILE | 9 | 15.018 | 31.488 | 41.770 | 1.00 18.85 | CPS5 |
| MOTA | 3790 | C | ILE | 9 | 14.538 | 29.012 | 46.121 | 1.00 20.96 | CPS5 |
| MOTA | 3791 | 0 | ILE | 9 | 13.482 | 28.392 | 45.964 | 1.00 20.30 | CPS5 |
| ATOM | 3792 | И | THR | 10 | 14.950 | 29.453 | 47.301 | 1.00 20.95 | CPS5 |
| ATOM | 3793 | CA | THR | 10 | 14.145 | 29.250 | 48.491 | 1.00 22.53 | CPS5 |
| ATOM | 3794 | CB | THR | 10 | 14.837 | 28.265 | 49.452 | 1.00 23.91 | CPS5 |
| ATOM | 3795 | | THR | 10 | 14.913 | 26.205 | 48.821 | 1.00 24.32 | CPS5 |
| ATOM | 3796 | CG2 | | 10 | 14.045 | 28.138 | 50.764 | 1.00 24.32 | CPS5 |
| ATOM | 3797 | C | THR | 10 | 13.893 | 30.567 | 49.207 | 1.00 23.06 | CPS5 |
| ATOM | 3798 | 0 | THR | 10 | 14.810 | 31.375 | 49.398 | 1.00 23.50 | CPS5 |
| ATOM | 3799 | N | GLU | 11 | 12.641 | 30.782 | 49.588 | 1.00 23.52 | CPSS |
| ATOM | 3800 | CA | GLU | 11 | 12.260 | 31.997 | 50.302 | 1.00 24.89 | CPS5 |
| ATOM | 3801 | CB | GLU | 11 | 10.747 | 32.212 | 50.168 | 1.00 25.23 | CPS5 |
| ATOM | 3801 | CG | GLU | 11 | 10.747 | 33.456 | 50.870 | 1.00 27.69 | CPS5 |
| ATOM | 3802 | CD | GLU | 11 | 8.701 | 33.491 | 50.901 | 1.00 29.32 | CPS5 |
| MOTA | 3804 | | GLU | 11 | 8.079 | 32.418 | 50.756 | 1.00 30.90 | CPS5 |
| MOTA | 3805 | | GLU | 11 | 8.129 | 34.584 | 51.089 | 1.00 33.76 | CPS5 |
| | | C | | 11 | 12.668 | 31.858 | 51.781 | 1.00 24.72 | CPS5 |
| MOTA | 3806 | | GLU | | 12.246 | 30.925 | 52.469 | 1.00 24.72 | CPS5 |
| ATOM | 3807 | 0 | GLU | 11 | | | 52.252 | 1.00 23.10 | CPS5 |
| ATOM | 3808 | N | LEU | 12 | 13.510 | 32.772 | | 1.00 24.83 | CPS5 |
| ATOM | 3809 | CA | LEU | 12 | 13.988 | 32.756 | 53.633 | 1.00 24.83 | CPS5 |
| ATOM | 3810 | CB | LEU | 12 | 14.850 | 33.997 | 53.895 | 1.00 28.80 | CPS5 |
| ATOM | 3811 | CG | LEU | 12 | 16.371 | 33.834 | 53.933 | | CPS5 |
| ATOM | 3812 | | LEU | 12 | 16.851 | 32.954 | 52.799 | 1.00 28.80 1.00 30.41 | CPS5 |
| ATOM | 3813 | | LEU | 12 | 17.018 | 35.199 | 53.858 | 1.00 30.41 | CPS5 |
| ATOM | 3814 | C | LEU | 12 | 12.856 | 32.691 | 54.661 | 1.00 25.34 | CPS5 |
| ATOM | 3815 | 0 | LEU | 12 | 12.947 | 31.983 | 55.658 | 1.00 25.34 | CPS5 |
| ATOM | 3816 | N | LYS | 13 | 11.788 | 33.432 | 54.403 | | CPS5 |
| ATOM | 3817 | CA | LYS | 13 | 10.644 | 33.479 | 55.304 | 1.00 29.15 | CPS5 |
| MOTA | 3818 | CB | LYS | 13 | 9.634 | 34.508 | 54.777 | 1.00 31.29 | CF3J |
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| ATOM | 3819 | CG | LYS | 13 | 8.429 | 34.734 | 55.668 | 1.00 36.36 | CPS5 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| MOTA | 3820 | CD | LYS | 13 | 7.596 | 35.907 | 55.154 | 1.00 40.04 | CPS5 |
| MOTA | 3821 | CE | LYS | 13 | 6.387 | 36.178 | 56.041 | 1.00 42.34 | CPS5 |
| MOTA | 3822 | NZ | LYS | 13 | 5.660 | 37.416 | 55.611 | 1.00 44.27 | CPS5 |
| MOTA | 3823 | С | LYS | 13 | 9.989 | 32.108 | 55.449 | 1.00 29.23 | CPS5 |
| MOTA | 3824 | 0 | LYS | 13 | 9.513 | 31.742 | 56.525 | 1.00 27.84 | CPS5 |
| MOTA | 3825 | N | ARG | 14 | 9.971 | 31.345 | 54.362 | 1.00 28.90 | CPS5 |
| ATOM | 3826 | CA | ARG | 14 | 9.371 | 30.019 | 54.384 | 1.00 29.32 | CPS5 |
| MOTA | 3827 | CB | ARG | 14 | 9.264 | 29.486 | 52.958 | 1.00 30.67 | CPS5 |
| MOTA | 3828 | CG | ARG | 14 | 8.489 | 28.186 | 52.828 | 1.00 33.67 | CPS5 |
| ATOM | 3829 | CD | ARG | 14 | 8.693 | 27.591 | 51.442 | 1.00 36.77 | CPS5 |
| ATOM | 3830 | NE | ARG | 14 | 8.435 | 26.157 | 51.442 | 1.00 40.83 | CPS5 |
| ATOM | 3831 | CZ | ARG | 14 | 9.204 | 25.259 | 50.836 | 1.00 42.06 | CPS5 |
| ATOM | 3832 | NHl | ARG | 14 | 10.289 | 25.640 | 50.176 | 1.00 40.50 | CPS5 |
| ATOM | 3833 | NH2 | ARG | 14 | 8.882 | 23.973 | 50.891 | 1.00 43.70 | CPS5 |
| ATOM | 3834 | С | ARG | 14 | 10.210 | 29.072 | 55.257 | 1.00 28.72 | CPS5 |
| MOTA | 3835 | 0 | ARG | 14 | 9.665 | 28.242 | 55.994 | 1.00 28.02 | CPS5 |
| MOTA | 3836 | N | ILE | 15 | 11.533 | 29.199 | 55.170 | 1.00 28.10 | CPS5 |
| MOTA | 3837 | CA | ILE | 15 | 12.439 | 28,378 | 55.972 | 1.00 27.56 | CPS5 |
| MOTA | 3838 | CB | ILE | 15 | 13.916 | 28.640 | 55.587 | 1.00 28.43 | CPS5 |
| MOTA | 3839 | CG2 | ILE | 15 | 14.863 | 28.021 | 56.623 | 1.00 27.74 | CPS5 |
| MOTA | 3840 | CG1 | | 15 | 14.201 | 28.042 | 54.204 | 1.00 26.73 | CPS5 |
| ATOM | 3841 | CD1 | ILE | 15 | 14.052 | 26.517 | 54.159 | 1.00 29.51 | CPS5 |
| ATOM | 3842 | С | ILE | 15 | 12.226 | 28.739 | 57.441 | 1.00 29.85 | CPS5 |
| ATOM | 3843 | 0 | ILE | 15 | 12.131 | 27.860 | 58.300 | 1.00 28.01 | CPS5 |
| ATOM | 3844 | N | ALA | 16 | 12.145 | 30.039 | 57.724 | 1.00 30.25 | CPS5 |
| ATOM | 3845 | CA | ALA | 16 | 11.929 | 30.508 | 59.097 | 1.00 31.84 | CPS5 |
| ATOM | 3846 | CB | ALA | 16 | 11.937 | 32.038 | 59.142 | 1.00 31.96 | CPS5 |
| ATOM | 3847 | С | ALA | 16 | 10.607 | 29.966 | 59.644 | 1.00 32.73 | CPS5 |
| ATOM | 3848 | Ō | ALA | 16 | 10.534 | 29.550 | 60.802 | 1.00 33.57 | CPS5 |
| ATOM | 3849 | N | SER | 17 | 9.564 | 29.958 | 58.820 | 1.00 33.10 | CPS5 |
| ATOM | 3850 | CA | SER | 17 | 8.276 | 29.435 | 59.269 | 1.00 35.41 | CPS5 |
| ATOM | 3851 | CB | SER | 17 | 7.206 | 29.639 | 58.201 | 1.00 36.49 | CPS5 |
| ATOM | 3852 | OG | SER | 17 | 6.988 | 31.024 | 57.990 | 1.00 40.91 | CPS5 |
| MOTA | 3853 | С | SER | 17 | 8.369 | 27.954 | 59.617 | 1.00 35.50 | CPS5 |
| ATOM | 3854 | 0 | SER | 17 | 7.938 | 27.532 | 60.696 | 1.00 35.16 | CPS5 |
| ATOM | 3855 | N | MET | 18 | 8.927 | 27.164 | 58.705 | 1.00 35.27 | CPS5 |
| ATOM | 3856 | CA | MET | 18 | 9.073 | 25.731 | 58.942 | 1.00 36.03 | CPS5 |
| ATOM | 3857 | CB | MET | 18 | 9.701 | 25.045 | 57.726 | 1.00 36.24 | CPS5 |
| ATOM | 3858 | CG | MET | 18 | 8.794 | 24.994 | 56.519 | 1.00 38.74 | CPS5 |
| ATOM | 3859 | SD | MET | 18 | 9.503 | 24.027 | 55.178 | 1.00 44.39 | CPS5 |
| MOTA | 3860 | CE | MET | 18 | 10.534 | 25.241 | 54.428 | 1.00 38.98 | CPS5 |
| MOTA | 3861 | С | MET | 18 | 9.918 | 25.462 | 60.180 | 1.00 35.92 | CPS5 |
| ATOM | 3862 | 0 | MET | 18 | 9.597 | 24.580 | 60.979 | 1.00 37.63 | CPS5 |
| ATOM | 3863 | N | ALA | 19 | 10.995 | 26.220 | 60.348 | 1.00 35.18 | CPS5 |
| MOTA | 3864 | CA | ALA | 19 | 11.859 | 26.033 | 61.504 | 1.00 35.87 | CPS5 |
| MOTA | 3865 | CB | ALA | 19 | 13.081 | 26.932 | 61.401 | 1.00 35.73 | CPS5 |
| MOTA | 3866 | C | ALA | 19 | 11.087 | 26.348 | 62.783 | 1.00 38.24 | CPS5 |
| ATOM | 3867 | 0 | ALA | 19 | 11.367 | 25.787 | 63.844 | 1.00 36.83 | CPS5 |
| ATOM | 3868 | N | GLY | 20 | 10.106 | 27.239 | 62.669 | 1.00 38.64 | CPS5 |
| ATOM | 3869 | CA | GLY | 20 | 9.320 | 27.619 | 63.827 | 1.00 40.77 | CPS5 |
| ATOM | 3870 | C | GLY | 20 | 8.203 | 26.663 | 64.196 | 1.00 41.91 | CPSS |
| ATOM | 3871 | ō | GLY | 20 | 7.826 | 26.580 | 65.361 | 1.00 43.62 | CPS5 |
| ATOM | 3872 | N | ARG | 21 | 7.668 | 25.935 | 63.225 | 1.00 42.69 | CPS5 |
| ATOM | 3873 | CA | ARG | 21 | 6.580 | 25.012 | 63.511 | | CPS5 |
| ATOM | 3874 | CB | ARG | 21 | 5.574 | 25.026 | 62.362 | 1.00 46.42 | CPS5 |
| ATOM | 3875 | CG | ARG | 21 | 6.018 | 24.224 | 61.156 | 1.00 50.19 | CPS5 |
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| ATOM | 3876 | CD | ARG | 21 | 5.388 | 24.747 | 59.879 | 1.00 53.16 | CPS5 |
|------|---------|-----|------|----|--------|--------|----------------|--------------------------|------|
| ATOM | 3877 | NE | ARG | 21 | 5.589 | 23.833 | 58.759 | 1.00 54.93 | CPS5 |
| MOTA | 3878 | CZ | ARG | 21 | 5.372 | 24.159 | 57.490 | 1.00 56.47 | CPS5 |
| MOTA | 3879 | NHl | ARG | 21 | 4.956 | 25.383 | 57.184 | 1.00 57.16 | CPS5 |
| MOTA | 3880 | NH2 | ARG | 21 | 5.554 | 23.258 | 56.533 | 1.00 56.82 | CPS5 |
| ATOM | 3881 | C | ARG | 21 | 7.051 | 23.579 | 63.753 | 1.00 44.27 | CPS5 |
| ATOM | 3882 | 0 | ARG | 21 | 6.367 | 22.803 | 64.420 | 1.00 44.45 | CPS5 |
| ATOM | 3883 | N | GLN | 22 | 8.213 | 23.226 | 63.209 | 1.00 42.85 | CPS5 |
| ATOM | 3884 | CA | GLN | 22 | 8.741 | 21.874 | 63.369 | 1.00 41.63 | CPS5 |
| ATOM | 3885 | CB | GLN | 22 | 9.212 | 21.351 | 62.011 | 1.00 41.96 | CPS5 |
| MOTA | 3886 | CG | GLN | 22 | 8.182 | 21.567 | 60.906 | 1.00 42.25 | CPS5 |
| ATOM | 3887 | CD | GLN | 22 | 8.610 | 21.008 | 59.560 | 1.00 44.24 | CPS5 |
| ATOM | 3888 | | GLN | 22 | 7.988 | 21.293 | 58.533 | 1.00 45.66 | CPS5 |
| ATOM | 3889 | | GLN | 22 | 9.664 | 20.202 | 59.557 | 1.00 42.69 | CPS5 |
| ATOM | 3890 | C | GLN | 22 | 9.882 | 21.862 | 64.387 | 1.00 41.06 | CPS5 |
| ATOM | 3891 | 0 | GLN | 22 | 10.853 | 22.607 | 64.255 | 1.00 41.24 | CPS5 |
| MOTA | 3892 | И | LYS | 23 | 9.764 | 20.995 | 65.390 | 1.00 39.60 | CPS5 |
| ATOM | 3893 | CA | LYS | 23 | 10.750 | 20.903 | 66.466 | 1.00 38.55 | CPS5 |
| ATOM | 3894 | CB | LYS | 23 | 10.730 | 19.695 | 67.357 | 1.00 39.83 | CPS5 |
| | | | | | | | | | CPS5 |
| ATOM | 3895 | CG | LYS | 23 | 11.370 | 19.589 | 68.551 | 1.00 41.79 1.00 43.79 | |
| ATOM | 3896 | CD | LYS | 23 | 10.771 | 18.745 | 69.654 | | CPS5 |
| ATOM | 3897 | CE | LYS | 23 | 10.448 | 17.353 | 69.161 | 1.00 44.48 | CPS5 |
| MOTA | 3898 | NZ | LYS | 23 | 10.028 | 16.518 | 70.294 | 1.00 46.17 | CPS5 |
| ATOM | 3899 | C | LYS | 23 | 12.236 | 20.885 | 66.106 | 1.00 37.06 | CPS5 |
| ATOM | 3900 | 0 | LYS | 23 | 12.982 | 21.787 | 66.501 | 1.00 40.33 | CPS5 |
| MOTA | 3901 | N | ARG | 24 | 12.679 | 19.862 | 65.389 | 1.00 32.83 | CPS5 |
| MOTA | 3902 | CA | ARG | 24 | 14.093 | 19.767 | 65.025 | 1.00 28.69 | CPS5 |
| ATOM | 3903 | CB | ARG | 24 | 14.693 | 18.448 | 65.537 | 1.00 27.47 | CPS5 |
| MOTA | 3904 | CG | ARG | 24 | 15.128 | 18.477 | 67.012 | 1.00 26.46 | CPS5 |
| MOTA | 3905 | CD | ARG | 24 | 15.742 | 17.141 | 67.435 | 1.00 26.25 | CPS5 |
| MOTA | 3906 | NE | ARG | 24 | 14.723 | 16.093 | 67.528 | 1.00 26.94 | CPS5 |
| ATOM | 3907 | CZ | ARG | 24 | 14.061 | 15.783 | 68.640 | 1.00 26.62 | CPS5 |
| ATOM | 3908 | | ARG | 24 | 14.304 | 16.423 | 69.781 | 1.00 28.42 | CPS5 |
| ATOM | 3909 | | ARG | 24 | 13.128 | 14.851 | 68.605 | 1.00 27.58 | CPS5 |
| MOTA | 3910 | С | ARG | 24 | 14.269 | 19.874 | 63.519 | 1.00 26.86 | CPS5 |
| MOTA | 3911 | 0 | ARG | 24 | 14.863 | 19.008 | 62.872 | 1.00 24.69 | CPS5 |
| MOTA | 3912 | N | PHE | 25 | 13.747 | 20.953 | 62.957 | 1.00 24.39 | CPS5 |
| MOTA | 3913 | CA | PHE | 25 | 13.848 | 21.148 | 61.515 | 1.00 24.06 | CPS5 |
| MOTA | 3914 | CB | PHE | 25 | 13.089 | 22.408 | 61.103 | 1.00 25.10 | CPS5 |
| ATOM | 3915 | CG | PHE | 25 | 13.220 | 22.738 | 59.645 | 1.00 25.01 | CPS5 |
| MOTA | 3916 | CD1 | PHE | 25 | 14.065 | 23.754 | 59.224 | 1.00 26.44 | CPS5 |
| MOTA | 3917 | CD2 | PHE | 25 | 12.502 | 22.029 | 58.69 5 | 1.00 26.17 | CPS5 |
| MOTA | 3918 | CE1 | PHE | 25 | 14.192 | 24.063 | 57.86 7 | 1.00 26.84 | CPS5 |
| ATOM | 3919 | CE2 | PHE | 25 | 12.624 | 22.330 | 57.338 | 1.00 27.83 | CPS5 |
| ATOM | 3920 | CZ | PHE | 25 | 13.470 | 23.348 | 56.929 | 1.00 26.25 | CPS5 |
| ATOM | 3921 | C | PHE | 25 | 15.289 | 21.241 | 61.034 | 1.00 23.02 | CPS5 |
| ATOM | 3922 | 0 | PHE | 25 | 15.669 | 20.583 | 60.067 | 1.00 23.63 | CPS5 |
| MOTA | 3923 | N | ALA | 26 | 16.096 | 22.055 | 61.702 | 1.00 21.62 | CPS5 |
| MOTA | 3924 | CA | ALA | 26 | 17.481 | 22.211 | 61.272 | 1.00 22.64 | CPS5 |
| MOTA | 3925 | CB | ALA | 26 | 18.200 | 23.213 | 62.171 | 1.00 21.17 | CPS5 |
| ATOM | 3926 | C | ALA | 26 | 18.203 | 20.868 | 61.295 | 1.00 22.18 | CPS5 |
| ATOM | 3927 | 0 | ALA | 26 | 18.962 | 20.542 | 60.382 | 1.00 21.14 | CPS5 |
| ATOM | 3928 | N | GLU | 27 | 17.967 | 20.098 | 62.356 | 1.00 21.95 | CPS5 |
| MOTA | 3929 | CA | GLU | 27 | 18.595 | 18.784 | 62.499 | 1.00 22.37 | CPS5 |
| ATOM | 3930 | CB | GLU | 27 | 18.231 | 18.176 | 63.862 | 1.00 21.57 | CPS5 |
| ATOM | 3931 | CG | GLU | 27 | 18.935 | 18.817 | 65.089 | 1.00 23.00 | CPS5 |
| ATOM | 3932 | CD | GLU | 27 | 18.465 | 20.233 | 65.452 | 1.00 24.81 | CPS5 |
| ALON | J J J Z | CD | 7110 | 41 | 20.403 | | | | |

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| ATOM | 3933 | OEl | GLU | 27 | 17.353 | 20.647 | 65.056 | 1.00 23.58 | CPS5 |
|------|------|---------|-----|----|------------------|--------|--------|------------|------|
| ATOM | 3934 | OE2 | GLU | 27 | 19.218 | 20.932 | 66.172 | 1.00 25.05 | CPS5 |
| ATOM | 3935 | C | GLU | 27 | 18.184 | 17.831 | 61.369 | 1.00 23.57 | CPS5 |
| ATOM | 3936 | 0 | GLU | 27 | 18.937 | 16.934 | 61.000 | 1.00 23.93 | CPS5 |
| MOTA | 3937 | N | ARG | 28 | 16.981 | 18.015 | 60.833 | 1.00 23.21 | CPS5 |
| MOTA | 3938 | CA | ARG | 28 | 16.502 | 17.173 | 59.742 | 1.00 25.30 | CPS5 |
| ATOM | 3939 | CB | ARG | 28 | 14.995 | 17.391 | 59.530 | 1.00 28.97 | CPS5 |
| ATOM | 3940 | CG | ARG | 28 | 14.413 | 16.636 | 58.327 | 1.00 31.14 | CPS5 |
| ATOM | 3941 | CD | ARG | 28 | 12.911 | 16.353 | 58.503 | 1.00 35.90 | CPS5 |
| ATOM | 3942 | NE | ARG | 28 | 12.063 | 17.535 | 58.340 | 1.00 36.29 | CPS5 |
| ATOM | 3943 | CZ | ARG | 28 | 11.774 | 18.089 | 57.165 | 1.00 38.49 | CPS5 |
| MOTA | 3944 | NH1 | | 28 | 12.264 | 17.571 | 56.045 | 1.00 37.03 | CPS5 |
| ATOM | 3945 | NH2 | | 28 | 10.980 | 19.154 | 57.105 | 1.00 38.67 | CPS5 |
| ATOM | 3946 | C | ARG | 28 | 17.245 | 17.488 | 58.439 | 1.00 24.41 | CPS5 |
| ATOM | 3947 | 0 | ARG | 28 | 17.582 | 16.596 | 57.666 | 1.00 24.06 | CPS5 |
| ATOM | 3948 | N | ILE | 29 | 17.517 | 18.765 | 58.218 | 1.00 23.36 | CPS5 |
| ATOM | 3949 | CA | ILE | 29 | 18.183 | 19.212 | 56.997 | 1.00 24.49 | CPS5 |
| ATOM | 3950 | CB | ILE | 29 | 17.817 | 20.693 | 56.704 | 1.00 24.90 | CPS5 |
| ATOM | 3951 | CG2 | ILE | 29 | 18.374 | 21.123 | 55.334 | 1.00 26.73 | CPS5 |
| ATOM | 3952 | | ILE | 29 | 16.305 | 20.880 | 56.773 | 1.00 24.80 | CPS5 |
| ATOM | 3953 | | ILE | 29 | 15.527 | 19.982 | 55.843 | 1.00 23.16 | CPS5 |
| ATOM | 3954 | C | ILE | 29 | 19.708 | 19.121 | 56.983 | 1.00 24.05 | CPS5 |
| ATOM | 3955 | 0 | ILE | 29 | 20.313 | 18.817 | 55.949 | 1.00 23.72 | CPS5 |
| ATOM | 3956 | N | LEU | 30 | 20.323 | 19.383 | 58.132 | 1.00 23.56 | CPS5 |
| MOTA | 3957 | CA | LEU | 30 | 21.778 | 19.444 | 58.240 | 1.00 23.33 | CPS5 |
| MOTA | 3958 | CB | LEU | 30 | 22.151 | 20.701 | 59.035 | 1.00 22.47 | CPS5 |
| ATOM | 3959 | CG | LEU | 30 | 21.503 | 22.020 | 58.591 | 1.00 23.18 | CPS5 |
| MOTA | 3960 | | LEU | 30 | 21.940 | 23.141 | 59.519 | 1.00 23.77 | CPS5 |
| ATOM | 3961 | | LEU | 30 | 21.901 | 22.348 | 57.157 | 1.00 22.19 | CPS5 |
| ATOM | 3962 | C | LEU | 30 | 22.492 | 18.238 | 58.854 | 1.00 24.18 | CPS5 |
| ATOM | 3963 | 0 | LEU | 30 | 21.966 | 17.577 | 59.753 | 1.00 24.62 | CPS5 |
| ATOM | 3964 | N | THR | 31 | 23.704 | 17.976 | 58.363 | 1.00 24.03 | CPS5 |
| ATOM | 3965 | CA | THR | 31 | 24.531 | 16.878 | 58.862 | 1.00 24.72 | CPS5 |
| ATOM | 3966 | CB | THR | 31 | 25.626 | 16.494 | 57.850 | 1.00 25.78 | CPS5 |
| ATOM | 3967 | | THR | 31 | 26.575 | 17.563 | 57.761 | 1.00 26.99 | CPS5 |
| ATOM | 3968 | CG2 | | 31 | 25.022 | 16.234 | 56.466 | 1.00 24.96 | CPS5 |
| MOTA | 3969 | C | THR | 31 | 25.228 | 17.351 | 60.140 | 1.00 24.37 | CPS5 |
| ATOM | 3970 | 0 | THR | 31 | 25.134 | 18.520 | 60.514 | 1.00 24.09 | CPS5 |
| ATOM | 3971 | И | ARG | 32 | 25.234 | 16.452 | 60.806 | 1.00 25.54 | CPS5 |
| ATOM | 3972 | CA | ARG | 32 | 26.642 | 16.832 | 62.031 | 1.00 27.17 | CPS5 |
| ATOM | 3973 | CB | ARG | 32 | 27.429 | 15.651 | 62.590 | 1.00 28.99 | CPS5 |
| ATOM | 3974 | CG | ARG | 32 | 26.583 | 14.597 | 63.261 | 1.00 31.34 | CPS5 |
| MOTA | 3975 | CD | ARG | 32 | 27.476 | 13.684 | 64.109 | 1.00 34.50 | CPS5 |
| ATOM | 3976 | NE | ARG | 32 | 26.701 | 12.698 | 64.853 | 1.00 38.58 | CPS5 |
| ATOM | 3977 | CZ | ARG | 32 | 27.200 | 11.916 | 65.809 | 1.00 40.34 | CPS5 |
| ATOM | 3978 | | ARG | 32 | 26.419 | 11.044 | 66.435 | 1.00 37.96 | CPS5 |
| | 3979 | | ARG | 32 | 28.480 | 12.009 | 66.145 | 1.00 42.21 | CPS5 |
| ATOM | | C | ARG | 32 | 27.589 | 18.014 | 61.865 | 1.00 27.70 | CPS5 |
| ATOM | 3980 | | | | 27.562 | 18.940 | 62.666 | 1.00 28.37 | CPS5 |
| ATOM | 3981 | O N | ARG | 32 | | 17.987 | 60.841 | 1.00 23.37 | CPS5 |
| MOTA | 3982 | N | SER | 33 | 28.439 29.379 | 19.088 | 60.652 | 1.00 27.37 | CPS5 |
| ATOM | 3983 | CA | SER | 33 | | 19.088 | 59.556 | 1.00 28.23 | CPS5 |
| ATOM | 3984 | CB | SER | 33 | 30.397 | | 58.309 | 1.00 30.14 | CPS5 |
| ATOM | 3985 | OG C | SER | 33 | 29.759 | 18.525 | | 1.00 34.75 | CPS5 |
| ATOM | 3986 | C | SER | 33 | 28.661 | 20.398 | 60.330 | 1.00 27.70 | CP35 |
| ATOM | 3987 | 0 | SER | 33 | 29.082 | 21.464 | 60.776 | 1.00 27.19 | CPS5 |
| MOTA | 3988 | N | GLU | 34 | 27.578 | 20.319 | 59.560 | 1.00 27.23 | CPS5 |
| MOTA | 3989 | CA | GLU | 34 | 26.804 | 21.511 | 59.212 | 1.00 47.47 | 0100 |
| | | | | | | | | | |

| ATOM | 3990 | CB | GLU | 34 | 25.759 | 21.171 | 58.148 | 1.00 27.07 | CPS5 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| | | | | | | | | | |
| MOTA | 3991 | CG | GLU | 34 | 26.368 | 20.872 | 56.783 | 1.00 28.76 | CPS5 |
| MOTA | 3992 | CD | GLU | 34 | 25.376 | 20.290 | 55.782 | 1.00 28.74 | CPS5 |
| MOTA | 3993 | OE1 | GLU | 34 | 25.664 | 20.350 | 54.569 | 1.00 31.36 | CPS5 |
| ATOM | 3994 | OE2 | GLU | 34 | 24.320 | 19.764 | 56.192 | 1.00 26.92 | CPS5 |
| MOTA | 3995 | С | GLU | 34 | 26.121 | 22.080 | 60.454 | 1.00 27.58 | CPS5 |
| ATOM | 3996 | 0 | GLU | 34 | 26.028 | 23.300 | 60.624 | 1.00 26.80 | CPS5 |
| ATOM | 3997 | N | LEU | 35 | 25.629 | 21.196 | 61.319 | 1.00 26.86 | CPS5 |
| MOTA | 3998 | CA | LEU | 35 | 24.988 | 21.653 | 62.545 | 1.00 27.86 | CPS5 |
| MOTA | 3999 | CB | LEU | 35 | 24.322 | 20.476 | 63.272 | 1.00 26.37 | CPS5 |
| | 4000 | | LEU | 35 | 23.004 | 19.992 | | 1.00 26.60 | CPS5 |
| ATOM | | CG | | | | | 62.650 | | |
| ATOM | 4001 | | LEU | 35 | 22.597 | 18.649 | 63.255 | 1.00 27.30 | CPS5 |
| MOTA | 4002 | CD2 | | 35 | 21.906 | 21.050 | 62.890 | 1.00 25.07 | CPS5 |
| MOTA | 4003 | С | LEU | 35 | 26.032 | 22.333 | 63.442 | 1.00 28.95 | CPS5 |
| MOTA | 4004 | 0 | LEU | 35 | 25.727 | 23.317 | 64.104 | 1.00 29.27 | CPS5 |
| MOTA | 4005 | N | ASP | 36 | 27.264 | 21.825 | 63.458 | 1.00 31.26 | CPS5 |
| MOTA | 4006 | CA | ASP | 36 | 28.306 | 22.453 | 64.279 | 1.00 33.66 | CPS5 |
| MOTA | 4007 | CB | ASP | 36 | 29.649 | 21.740 | 64.127 | 1.00 36.86 | CPS5 |
| ATOM | 4008 | CG | ASP | 36 | 29.668 | 20.386 | 64.795 | 1.00 39.66 | CPS5 |
| ATOM | 4009 | OD1 | ASP | 36 | 28.990 | 20.235 | 65.833 | 1.00 43.45 | CPS5 |
| ATOM | 4010 | | ASP | 36 | 30.373 | 19.479 | 64.297 | 1.00 41.30 | CPS5 |
| ATOM | 4011 | C | ASP | 36 | 28.481 | 23.905 | 63.871 | 1.00 34.39 | CPS5 |
| ATOM | 4012 | 0 | ASP | 36 | 28.608 | 24.794 | 64.722 | 1.00 34.60 | CPS5 |
| | | | | 37 | 28.488 | 24.734 | 62.563 | 1.00 33.83 | CPS5 |
| MOTA | 4013 | N | GLN | | | | | 1.00 35.12 | CPS5 |
| ATOM | 4014 | CA | GLN | 37 | 28.639 | 25.483 | 62.015 | | |
| MOTA | 4015 | CB | GLN | 37 | 28.809 | 25.394 | 60.499 | 1.00 36.30 | CPS5 |
| MOTA | 4016 | CG | GLN | 37 | 30.079 | 24.660 | 60.055 | 1.00 41.36 | CPS5 |
| ATOM | 4017 | CD | GLN | 37 | 29.944 | 24.026 | 58.676 | 1.00 43.00 | CPS5 |
| ATOM | 4018 | OE1 | GLN | 37 | 29.434 | 24.646 | 57.746 | 1.00 44.80 | CPS5 |
| MOTA | 4019 | NE2 | GLN | 37 | 30.408 | 22.786 | 58.541 | 1.00 44.26 | CPS5 |
| MOTA | 4020 | C | GLN | 37 | 27.409 | 26.328 | 62.344 | 1.00 34.18 | CPS5 |
| MOTA | 4021 | 0 | GLN | 37 | 27.513 | 27.470 | 62.794 | 1.00 33.82 | CPS5 |
| MOTA | 4022 | N | TYR | 38 | 26.240 | 25.736 | 62.126 | 1.00 32.84 | CPS5 |
| ATOM | 4023 | CA | TYR | 38 | 24.963 | 26.395 | 62.349 | 1.00 32.66 | CPS5 |
| ATOM | 4024 | CB | TYR | 38 | 23.846 | 25.419 | 61.961 | 1.00 29.71 | CPS5 |
| ATOM | 4025 | CG | TYR | 38 | 22.433 | 25.884 | 62.224 | 1.00 29.29 | CPS5 |
| ATOM | 4026 | | TYR | 38 | 21.721 | 25.404 | 63.317 | 1.00 29.80 | CPS5 |
| | 4027 | | TYR | 38 | 20.401 | 25.776 | 63.541 | 1.00 31.00 | CPS5 |
| ATOM | | | | | | 26.763 | 61.355 | 1.00 28.96 | CPS5 |
| MOTA | 4028 | | TYR | 38 | 21.788 | | | 1.00 28.65 | CPS5 |
| MOTA | 4029 | | TYR | 38 | 20.459 | 27.146 | 61.571 | | CPS5 |
| ATOM | 4030 | cz | TYR | 38 | 19.776 | 26.644 | 62.665 | 1.00 29.30 | CPS5 |
| MOTA | 4031 | OH | TYR | 38 | 18.462 | 26.985 | 62.885 | 1.00 28.92 | |
| ATOM | 4032 | C | TYR | 38 | 24.746 | 26.939 | 63.765 | 1.00 34.02 | CPS5 |
| MOTA | 4033 | 0 | TYR | 38 | 24.292 | 28.068 | 63.936 | 1.00 34.37 | CPS5 |
| MOTA | 4034 | N | TYR | 39 | 25.076 | 26.154 | 64.780 | 1.00 36.23 | CPS5 |
| MOTA | 4035 | CA | TYR | 39 | 24.860 | 26.613 | 66.144 | 1.00 38.88 | CPS5 |
| ATOM | 4036 | CB | TYR | 39 | 24.762 | 25.414 | 67.082 | 1.00 38.30 | CPS5 |
| ATOM | 4037 | CG | TYR | 39 | 23.371 | 24.847 | 67.036 | 1.00 38.06 | CPS5 |
| ATOM | 4038 | CD1 | TYR | 39 | 22.273 | 25.658 | 67.338 | 1.00 38.93 | CPS5 |
| ATOM | 4039 | | TYR | 39 | 20.974 | 25.194 | 67.203 | 1.00 39.58 | CPS5 |
| MOTA | 4040 | | TYR | 39 | 23.134 | 23.546 | 66.608 | 1.00 37.49 | CPS5 |
| | = | | TYR | 39 | 21.837 | 23.064 | 66.469 | 1.00 37.88 | CPS5 |
| MOTA | 4041 | | | | 20.760 | 23.893 | 66.763 | 1.00 39.42 | CPS5 |
| MOTA | 4042 | CZ | TYR | 39 | | | | 1.00 38.55 | CPS5 |
| ATOM | 4043 | OH | TYR | 39 | 19.470 | 23.450 | 66.592 | 1.00 38.33 | CPS5 |
| ATOM | 4044 | С | TYR | 39 | 25.816 | 27.658 | 66.692 | | CPS5 |
| ATOM | 4045 | 0 | TYR | 39 | 25.662 | 28.109 | 67.822 | 1.00 42.90 | |
| MOTA | 4046 | N | GLU | 40 | 26.789 | 28.060 | 65.887 | 1.00 43.80 | CPS5 |
| | | | | | | | | | |

| A TOM | 4047 | CA | GLU | 40 | 27.731 | 29.090 | 66.304 | 1.00 46.08 | CDCC |
|-------|------|-----|-------|----|--------|--------|--------|------------|------|
| ATOM | 4047 | | | | | | | | CPS5 |
| MOTA | 4048 | CB | GLU | 40 | 29.140 | 28.737 | 65.834 | 1.00 48.41 | CPS5 |
| MOTA | 4049 | CG | GLU | 40 | 29.806 | 27.639 | 66.639 | 1.00 52.50 | CPS5 |
| MOTA | 4050 | CD | GLU | 40 | 31.155 | 27.248 | 66.063 | 1.00 54.95 | CPS5 |
| ATOM | 4051 | | GLU | 40 | 31.969 | 28.154 | 65.774 | 1.00 56.23 | CPS5 |
| MOTA | 4052 | OE2 | GLU | 40 | 31.403 | 26.033 | 65.904 | 1.00 57.17 | CPS5 |
| ATOM | 4053 | C | GLU | 40 | 27.322 | 30.446 | 65.721 | 1.00 46.24 | CPS5 |
| MOTA | 4054 | 0 | GLU | 40 | 27.932 | 31.475 | 66.023 | 1.00 46.47 | CPS5 |
| MOTA | 4055 | N | LEU | 41 | 26.279 | 30.443 | 64.896 | 1.00 45.08 | CPS5 |
| ATOM | 4056 | CA | LEU | 41 | 25.803 | 31.664 | 64.254 | 1.00 44.90 | CPS5 |
| ATOM | 4057 | CB | LEU | 41 | 25.304 | 31.348 | 62.840 | 1.00 44.02 | CPS5 |
| ATOM | 4058 | CG | LEU | 41 | 26.227 | 30.623 | 61.859 | 1.00 43.61 | CPS5 |
| ATOM | 4059 | | LEU | 41 | 25.443 | 30.306 | 60.591 | 1.00 42.67 | CPS5 |
| | | | | | 27.439 | 31.480 | 61.530 | 1.00 43.84 | CPS5 |
| ATOM | 4060 | | LEU | 41 | | | | | |
| MOTA | 4061 | C | LEU | 41 | 24.685 | 32.376 | 65.013 | 1.00 45.61 | CPS5 |
| MOTA | 4062 | 0 | LEU | 41 | 24.021 | 31.789 | 65.869 | 1.00 45.79 | CPS5 |
| MOTA | 4063 | N | SER | 42 | 24.479 | 33.648 | 64.677 | 1.00 46.42 | CPS5 |
| ATOM | 4064 | CA | SER | 42 | 23.432 | 34.456 | 65.288 | 1.00 47.43 | CPS5 |
| ATOM | 4065 | CB | SER | 42 | 23.615 | 35.924 | 64.915 | 1.00 48.22 | CPS5 |
| ATOM | 4066 | OG | SER | 42 | 23.440 | 36.106 | 63.520 | 1.00 48.72 | CPS5 |
| ATOM | 4067 | C | SER | 42 | 22.105 | 33.963 | 64.734 | 1.00 47.92 | CPS5 |
| MOTA | 4068 | 0 | SER | 42 | 22.081 | 33.205 | 63.763 | 1.00 47.71 | CPS5 |
| MOTA | 4069 | N | GLU | 43 | 21.000 | 34.399 | 65.328 | 1.00 48.18 | CPS5 |
| ATOM | 4070 | CA | GLU | 43 | 19.689 | 33.959 | 64.861 | 1.00 48.69 | CPS5 |
| ATOM | 4071 | CB | GLU | 43 | 18.581 | 34.563 | 65.728 | 1.00 50.88 | CPS5 |
| ATOM | 4072 | CG | GLU | 43 | 17.286 | 33.765 | 65.683 | 1.00 53.85 | CPS5 |
| ATOM | 4073 | CD | GLU | 43 | 16.099 | 34.579 | 65.201 | 1.00 56.30 | CPS5 |
| ATOM | 4074 | | GLU | 43 | 16.189 | 35.176 | 64.105 | 1.00 57.99 | CPS5 |
| | | OE2 | | 43 | 15.073 | 34.614 | 65.916 | 1.00 56.86 | CPS5 |
| MOTA | 4075 | | GLU | 43 | 19.449 | 34.308 | 63.389 | 1.00 47.59 | CPS5 |
| MOTA | 4076 | C | | | | | | 1.00 47.33 | CPS5 |
| MOTA | 4077 | 0 | GLU | 43 | 18.899 | 33.503 | 62.635 | | CPS5 |
| ATOM | 4078 | N | LYS | 44 | 19.861 | 35.504 | 62.979 | 1.00 46.55 | |
| ATOM | 4079 | CA | LYS | 44 | 19.680 | 35.926 | 61.591 | 1.00 46.07 | CPS5 |
| ATOM | 4080 | CB | LYS | 44 | 19.973 | 37.422 | 61.439 | 1.00 47.29 | CPS5 |
| ATOM | 4081 | CG | LYS | 44 | 19.730 | 37.935 | 60.031 | 1.00 49.35 | CPS5 |
| MOTA | 4082 | CD | LYS | 44 | 20.148 | 39.384 | 59.857 | 1.00 50.89 | CPS5 |
| MOTA | 4083 | CE | LYS | 44 | 19.837 | 39.855 | 58.440 | 1.00 52.29 | CPS5 |
| MOTA | 4084 | NZ | LYS | 44 | 20.265 | 41.261 | 58.188 | 1.00 53.26 | CPS5 |
| ATOM | 4085 | C | LYS | 44 | 20.597 | 35.130 | 60.660 | 1.00 44.52 | CPS5 |
| ATOM | 4086 | 0 | LYS | 44 | 20.185 | 34.698 | 59.579 | 1.00 43.62 | CPS5 |
| MOTA | 4087 | N | ARG | 45 | 21.842 | 34.944 | 61.084 | 1.00 42.61 | CPS5 |
| ATOM | 4088 | CA | ARG | 45 | 22.816 | 34.195 | 60.297 | 1.00 41.42 | CPS5 |
| MOTA | 4089 | CB | ARG | 45 | 24.193 | 34.284 | 60.957 | 1.00 43.69 | CPS5 |
| MOTA | 4090 | CG | ARG | 45 | 25.001 | 35.512 | 60.552 | 1.00 47.18 | CPS5 |
| MOTA | 4091 | CD | ARG | 45 | 26.039 | 35.120 | 59.517 | 1.00 50.46 | CPS5 |
| ATOM | 4092 | NE | ARG | 45 | 25.455 | 34.243 | 58.506 | 1.00 53.21 | CPS5 |
| ATOM | 4093 | CZ | ARG | 45 | 26.141 | 33.355 | 57.794 | 1.00 54.22 | CPS5 |
| ATOM | 4094 | | . ARG | 45 | 27.450 | 33.219 | 57.975 | 1.00 54.73 | CPS5 |
| | 4095 | | ARG | 45 | 25.514 | 32.593 | 56.909 | 1.00 54.37 | CPS5 |
| ATOM | | | ARG | 45 | 22.385 | 32.735 | 60.156 | 1.00 39.25 | CPS5 |
| MOTA | 4096 | C | | | | | 59.128 | 1.00 37.24 | CPS5 |
| MOTA | 4097 | 0 | ARG | 45 | 22.620 | 32.100 | 61.196 | 1.00 37.24 | CPS5 |
| MOTA | 4098 | N | LYS | 46 | 21.748 | 32.209 | | 1.00 36.43 | CPS5 |
| ATOM | 4099 | CA | LYS | 46 | 21.273 | 30.830 | 61.175 | | CPS5 |
| ATOM | 4100 | CB | LYS | 46 | 20.618 | 30.472 | 62.511 | 1.00 34.58 | |
| MOTA | 4101 | CG | LYS | 46 | 21.608 | 30.164 | | 1.00 35.23 | CPS5 |
| MOTA | 4102 | CD | LYS | 46 | 20.871 | 29.751 | | 1.00 37.58 | CPS5 |
| MOTA | 4103 | CE | LYS | 46 | 21.842 | 29.392 | 66.010 | 1.00 39.36 | CPS5 |

| MOTA | 4104 | NZ | LYS | 46 | 21.100 | 29.022 | 67.241 | 1.00 40.50 | CPS5 |
|------|------|-----|-----|----------|--------|--------|--------|------------|-------|
| MOTA | 4105 | C | LYS | 46 | 20.267 | 30.612 | 60.047 | 1.00 33.30 | CPS5 |
| MOTA | 4106 | 0 | LYS | 46 | 20.350 | 29.631 | 59.310 | 1.00 31.70 | CPS5 |
| MOTA | 4107 | N | ASN | 47 | 19.313 | 31.531 | 59.924 | 1.00 31.25 | CPS5 |
| ATOM | 4108 | CA | ASN | 47 | 18.295 | 31.424 | 58.892 | 1.00 30.79 | CPS5 |
| ATOM | 4109 | CB | NZA | 47 | 17.298 | 32.575 | 59.020 | 1.00 32.61 | CPS5 |
| ATOM | 4110 | CG | ASN | 47 | 16.216 | 32.532 | 57.963 | 1.00 33.88 | CPS5 |
| ATOM | 4111 | OD1 | ASN | 47 | 15.427 | 31.588 | 57.896 | 1.00 34.99 | CPS5 |
| ATOM | 4112 | ND2 | ASN | 47 | 16.176 | 33.558 | 57.121 | 1.00 36.56 | CPS5 |
| ATOM | 4113 | C | ASN | 47 | 18.944 | 31.440 | 57.513 | 1.00 31.05 | CPS5 |
| ATOM | 4114 | 0 | ASN | 47 | 18.588 | 30.637 | 56.648 | 1.00 30.48 | CPS5 |
| ATOM | 4115 | N | GLU | 48 | 19.888 | 32.358 | 57.311 | 1.00 28.97 | CPS5 |
| ATOM | 4116 | CA | GLU | 48 | 20.588 | 32.468 | 56.031 | 1.00 29.63 | CPS5 |
| ATOM | 4117 | CB | GLU | 48 | 21.570 | 33.640 | 56.061 | 1.00 23.85 | CPS5 |
| ATOM | 4118 | CG | GLU | 48 | 20.921 | 34.975 | 56.372 | 1.00 37.62 | CPS5 |
| ATOM | 4119 | CD | GLU | 48 | 21.936 | 36.092 | 56.540 | 1.00 40.25 | CPS5 |
| ATOM | 4120 | | GLU | 48 | 21.536 | 37.217 | 56.898 | | |
| MOTA | 4121 | | GLU | 48 | 23.141 | 35.845 | 56.313 | 1.00 42.86 | CPS5 |
| | | | | | | | | 1.00 41.40 | CPS5 |
| ATOM | 4122 | C | GLU | 48 | 21.358 | 31.187 | 55.726 | 1.00 27.51 | CPS5 |
| ATOM | 4123 | 0 | GLU | 48 | 21.281 | 30.644 | 54.622 | 1.00 26.82 | CPS5 |
| ATOM | 4124 | N | PHE | 49 | 22.106 | 30.712 | 56.711 | 1.00 25.07 | CPS5 |
| ATOM | 4125 | CA | PHE | 49 | 22.886 | 29.497 | 56.552 | 1.00 25.50 | CPS5 |
| ATOM | 4126 | CB | PHE | 49 | 23.636 | 29.194 | 57.844 | 1.00 25.32 | CPS5 |
| ATOM | 4127 | CG | PHE | 49 | 24.519 | 27.986 | 57.765 | 1.00 26.38 | CPS5 |
| ATOM | 4128 | | PHE | 49 | 25.798 | 28.077 | 57.233 | 1.00 27.15 | CPS5 |
| ATOM | 4129 | | PHE | 49 | 24.080 | 26.757 | 58.249 | 1.00 24.90 | CPS5 |
| ATOM | 4130 | | PHE | 49 | 26.640 | 26.954 | 57.189 | 1.00 28.06 | CPS5 |
| ATOM | 4131 | | PHE | 49 | 24.903 | 25.635 | 58.211 | 1.00 25.87 | CPS5 |
| MOTA | 4132 | CZ | PHE | 49 | 26.195 | 25.736 | 57.678 | 1.00 26.35 | CPS5 |
| ATOM | 4133 | C | PHE | 49 | 21.991 | 28.312 | 56.203 | 1.00 24.96 | CPS5 |
| MOTA | 4134 | 0 | PHE | 49 | 22.255 | 27.581 | 55.248 | 1.00 24.24 | CPS5 |
| MOTA | 4135 | И | LEU | 50 | 20.939 | 28.114 | 56.995 | 1.00 23.68 | CPS5 |
| MOTA | 4136 | CA | LEU | 50 | 20.024 | 27.005 | 56.773 | 1.00 23.00 | CPS5 |
| ATOM | 4137 | CB | LEU | 50 | 18.974 | 26.962 | 57.892 | 1.00 24.58 | CPS5 |
| ATOM | 4138 | CG | LEU | 50 | 17.860 | 25.903 | 57.864 | 1.00 24.45 | CPS5 |
| ATOM | 4139 | CD1 | LEU | 50 | 18.431 | 24.483 | 57.785 | 1.00 24.94 | CPS5 |
| ATOM | 4140 | CD2 | LEU | 50 | 17.022 | 26.072 | 59.142 | 1.00 23.53 | CPS5 |
| ATOM | 4141 | C | LEU | 50 | 19.349 | 27.082 | 55.403 | 1.00 22.61 | CPS5 |
| ATOM | 4142 | 0 | LEU | 50 | 19.268 | 26.083 | 54.693 | 1.00 21.59 | CPS5 |
| ATOM | 4143 | N | ALA | 51 | 18.865 | 28.260 | 55.021 | 1.00 21.89 | CPS5 |
| ATOM | 4144 | CA | ALA | 51 | 18.213 | 28.390 | 53.723 | 1.00 21.84 | CPS5 |
| ATOM | 4145 | CB | ALA | 51 | 17.637 | 29.799 | 53.556 | 1.00 21.05 | CPS5 |
| MOTA | 4146 | С | ALA | 51 | 19.191 | 28.076 | 52.585 | 1.00 21.23 | CPS5 |
| MOTA | 4147 | 0 | ALA | 51 | 18.813 | 27.458 | 51.587 | 1.00 21.60 | CPS5 |
| MOTA | 4148 | N | GLY | 52 | 20.442 | 28.506 | 52.734 | 1.00 21.20 | CPS5 |
| MOTA | 4149 | CA | GLY | 52 | 21.437 | 28.245 | 51.700 | 1.00 21.20 | CPS5 |
| MOTA | 4150 | С | GLY | 52 | 21.769 | 26.767 | 51.563 | 1.00 22.06 | CPS5 |
| ATOM | 4151 | 0 | GLY | 52 | 21.929 | 26.252 | 50.452 | 1.00 20.70 | CPS5 |
| ATOM | 4152 | N | ARG | 53 | 21.888 | 26.074 | 52.693 | 1.00 21.88 | CPS5 |
| ATOM | 4153 | CA | ARG | 53 | 22.188 | 24.645 | 52.659 | 1.00 21.58 | CPS5 |
| ATOM | 4154 | CB | ARG | 53 | 22.565 | 24.152 | 54.065 | 1.00 23.65 | CPS5 |
| ATOM | 4155 | CG | ARG | 53 | 24.066 | 24.127 | 54.329 | 1.00 27.20 | CPS5 |
| ATOM | 4156 | CD | ARG | 53 | 24.751 | 25.409 | 53.912 | 1.00 30.18 | CPS5 |
| ATOM | 4157 | NE | ARG | 53 | 26.181 | 25.365 | 54.194 | 1.00 32.58 | CPS5 |
| ATOM | 4158 | CZ | ARG | 53 | 27.072 | 26.204 | 53.677 | 1.00 35.33 | CPS5 |
| | 4158 | | ARG | 53 53 | 26.690 | 27.163 | 52.836 | 1.00 37.77 | CPS5 |
| ATOM | | | | | | | 54.006 | 1.00 37.77 | CPS5 |
| ATOM | 4160 | NH2 | ARG | 53 | 28.350 | 26.089 | 34.000 | 1.00 37.90 | (: 0) |

| MOTA | 4161 | С | ARG | 53 | 20.976 | 23.890 | 52.125 | 1.00 21.40 | CPS5 |
|--------------|------|-----|-----|------------|--------|--------|--------|------------|------|
| MOTA | 4162 | 0 | ARG | 53 | 21.106 | 22.921 | 51.365 | 1.00 20.53 | CPS5 |
| ATOM | 4163 | N | PHE | 54 | 19.795 | 24.341 | 52.528 | 1.00 19.73 | CPS5 |
| MOTA | 4164 | CA | PHE | 54 | 18.548 | 23.745 | 52.070 | 1.00 19.35 | CPS5 |
| MOTA | 4165 | CB | PHE | 54 | 17.364 | 24.482 | 52.724 | 1.00 19.38 | CPS5 |
| ATOM | 4166 | CG | PHE | 54 | 16.023 | 23.926 | 52.353 | 1.00 20.72 | CPS5 |
| ATOM | 4167 | CD1 | PHE | 54 | 15.330 | 24.414 | 51.245 | 1.00 22.15 | CPS5 |
| MOTA | 4168 | CD2 | PHE | 54 | 15.448 | 22.903 | 53.107 | 1.00 21.41 | CPS5 |
| ATOM | 4169 | CE1 | PHE | 54 | 14.080 | 23.891 | 50.893 | 1.00 22.91 | CPS5 |
| ATOM | 4170 | CE2 | PHE | 54 | 14.196 | 22.371 | 52.762 | 1.00 22.41 | CPS5 |
| MOTA | 4171 | CZ | PHE | 54 | 13.513 | 22.868 | 51.654 | 1.00 22.38 | CPS5 |
| ATOM | 4172 | С | PHE | 54 | 18.484 | 23.873 | 50.537 | 1.00 19.62 | CPS5 |
| ATOM | 4173 | Ō | PHE | 54 | 18.223 | 22.901 | 49.821 | 1.00 18.89 | CPS5 |
| MOTA | 4174 | N | ALA | 55 | 18.736 | 25.082 | 50.046 | 1.00 19.98 | CPS5 |
| ATOM | 4175 | CA | ALA | 55 | 18.690 | 25.348 | 48.608 | 1.00 19.92 | CPS5 |
| ATOM | 4176 | CB | ALA | 55 | 18.930 | 26.839 | 48.347 | 1.00 18.81 | CPS5 |
| MOTA | 4177 | C | ALA | 55 | 19.721 | 24.515 | 47.859 | 1.00 19.28 | CPS5 |
| ATOM | 4178 | 0 | ALA | 55 | 19.442 | 23.972 | 46.788 | 1.00 19.25 | CPS5 |
| ATOM | 4179 | N | ALA | 56 | 20.916 | 24.398 | 48.422 | 1.00 19.74 | CPS5 |
| ATOM | 4180 | CA | ALA | 56 | 21.954 | 23.621 | 47.755 | 1.00 20.82 | CPS5 |
| ATOM | 4181 | CB | ALA | 56 | 23.299 | 23.838 | 48.446 | 1.00 20.78 | CPS5 |
| ATOM | 4182 | C | ALA | 56 | 21.622 | 22.130 | 47.693 | 1.00 20.48 | CPS5 |
| ATOM | 4183 | ō | ALA | 56 | 21.944 | 21.459 | 46.702 | 1.00 20.22 | CPSS |
| ATOM | 4184 | N | LYS | 57 | 20.993 | 21.600 | 48.746 | 1.00 19.44 | CPS5 |
| ATOM | 4185 | CA | LYS | 57 | 20.642 | 20.187 | 48.754 | 1.00 19.12 | CPS5 |
| ATOM | 4186 | CB | LYS | 5 <i>7</i> | 20.336 | 19.718 | 50.191 | 1.00 18.95 | CPS5 |
| ATOM | 4187 | CG | LYS | 57 | 21.571 | 19.809 | 51.077 | 1.00 18.78 | CPS5 |
| ATOM | 4188 | CD | LYS | 57 | 21.395 | 19.116 | 52.429 | 1.00 22.43 | CPS5 |
| ATOM | 4189 | CE | LYS | 57 | 22.575 | 19.458 | 53.329 | 1.00 22.68 | CPS5 |
| ATOM | 4190 | NZ | LYS | 57 57 | 22.712 | 18.541 | 54.502 | 1.00 21.60 | CPS5 |
| ATOM | 4191 | C | LYS | 57 | 19.465 | 19.937 | 47.821 | 1.00 20.77 | CPS5 |
| ATOM | 4192 | 0 | LYS | 57 | 19.401 | 18.900 | 47.160 | 1.00 20.15 | CPS5 |
| MOTA | 4193 | И | GLU | 58 | 18.535 | 20.885 | 47.757 | 1.00 19.45 | CPS5 |
| ATOM | 4194 | CA | GLU | 58 | 17.410 | 20.738 | 46.845 | 1.00 21.16 | CPS5 |
| ATOM | 4195 | CB | GLU | 58 | 16.409 | 21.887 | 47.020 | 1.00 21.14 | CPS5 |
| ATOM | 4196 | CG | GLU | 58 | 15.520 | 21.769 | 48.247 | 1.00 25.24 | CPS5 |
| MOTA | 4197 | CD | GLU | 58 | 14.558 | 20.505 | 48.153 | 1.00 29.18 | CPS5 |
| ATOM | 4198 | | GLU | 58 | 14.482 | 19.993 | 47.066 | 1.00 31.68 | CPS5 |
| ATOM | 4199 | | GLU | 58 | 13.875 | 20.305 | 49.156 | 1.00 29.87 | CPS5 |
| ATOM | 4200 | C | GLU | 58 | 17.943 | 20.741 | 45.410 | 1.00 20.35 | CPS5 |
| ATOM | 4201 | 0 | GLU | 58 | 17.543 | 19.908 | 44.590 | 1.00 20.00 | CPS5 |
| ATOM | 4201 | N | ALA | 59 | 18.848 | 21.675 | 45.113 | 1.00 20.46 | CPS5 |
| | 4202 | CA | ALA | 59 | 19.418 | | 43.769 | | CPS5 |
| ATOM | 4204 | CB | ALA | 59 | 20.353 | | 43.655 | 1.00 20.63 | CPS5 |
| ATOM ATOM | 4204 | C | ALA | 59 | 20.175 | | | 1.00 20.79 | CPS5 |
| | 4205 | 0 | ALA | 59 | 20.104 | | 42.312 | 1.00 20.80 | CPS5 |
| ATOM ATOM | 4206 | N | PHE | 60 | 20.104 | 19.965 | 44.404 | 1.00 19.71 | CPS5 |
| | 4207 | CA | PHE | 60 | 21.643 | | 44.153 | 1.00 19.50 | CPS5 |
| ATOM | | | PHE | 60 | 22.511 | | 45.361 | 1.00 20.28 | CPS5 |
| MOTA | 4209 | CB | PHE | 60 | 23.252 | | | 1.00 22.22 | CPS5 |
| MOTA | 4210 | CG | | 60 | 24.498 | | 44.548 | | CPS5 |
| ATOM | 4211 | | PHE | | | | 45.538 | 1.00 23.50 | CPS5 |
| ATOM | 4212 | | PHE | 60 60 | 22.657 | | 44.285 | 1.00 25.08 | CPS5 |
| MOTA | 4213 | | PHE | 60 60 | 25.145 | | | 1.00 26.22 | CPS5 |
| ATOM | 4214 | | PHE | 60 | 23.287 | | | | CPS5 |
| ATOM | 4215 | CZ | PHE | 60 | 24.534 | | | | CPS5 |
| MOTA | 4216 | C | PHE | 60 | 20.665 | | | | CPS5 |
| ATOM | 4217 | 0 | PHE | 60 | 20.893 | 10.1/4 | 74.340 | 1.00 20.70 | 0 |
| | | | | | | | | | |

| ATOM | 4218 | N | SER | 61 | 19.575 | 17.530 | 44.615 | 1.00 19.93 | CPS5 |
|--------|------|-----|-----|----|--------|--------|--------|------------|------|
| ATOM | 4219 | CA | SER | 61 | 18.596 | 16.461 | 44.437 | 1.00 22.05 | CPS5 |
| ATOM | 4220 | CB | SER | 61 | 17.542 | 16.505 | 45.550 | 1.00 21.89 | CPS5 |
| MOTA | 4221 | OG | SER | 61 | 16.571 | 17.505 | 45.308 | 1.00 22.40 | CPS5 |
| ATOM | 4222 | C | SER | 61 | 17.931 | 16.519 | 43.067 | 1.00 22.70 | CPS5 |
| ATOM | 4223 | 0 | SER | 61 | 17.482 | 15.494 | 42.540 | 1.00 23.10 | CPS5 |
| ATOM | 4224 | N | LYS | 62 | 17.874 | 17.716 | 42.487 | 1.00 21.75 | CPS5 |
| ATOM | 4225 | CA | LYS | 62 | 17.292 | 17.888 | 41.158 | 1.00 22.11 | CPS5 |
| | | | | | | | | | |
| ATOM | 4226 | CB | LYS | 62 | 16.914 | 19.349 | 40.932 | 1.00 23.25 | CPS5 |
| MOTA | 4227 | ÇG | LYS | 62 | 15.636 | 19.790 | 41.661 | 1.00 26.97 | CPS5 |
| MOTA | 4228 | CD | LYS | 62 | 15.515 | 21.316 | 41.597 | 1.00 29.60 | CPS5 |
| ATOM | 4229 | CE | LYS | 62 | 14.085 | 21.787 | 41.383 | 1.00 33.49 | CPS5 |
| MOTA | 4230 | NZ | LYS | 62 | 13.174 | 21.402 | 42.470 | 1.00 35.09 | CPS5 |
| ATOM | 4231 | C | LYS | 62 | 18.290 | 17.431 | 40.095 | 1.00 22.61 | CPS5 |
| ATOM | 4232 | 0 | LYS | 62 | 17.897 | 16.841 | 39.079 | 1.00 22.72 | CPS5 |
| ATOM | 4233 | N | ALA | 63 | 19.577 | 17.695 | 40.333 | 1.00 21.05 | CPS5 |
| MOTA | 4234 | CA | ALA | 63 | 20.627 | 17.283 | 39.408 | 1.00 21.93 | CPS5 |
| MOTA | 4235 | CB | ALA | 63 | 21.965 | 17.909 | 39.801 | 1.00 21.40 | CPS5 |
| ATOM | 4236 | C | ALA | 63 | 20.737 | 15.767 | 39.476 | 1.00 23.26 | CPS5 |
| | | | | | | 15.113 | | 1.00 23.20 | CPS5 |
| ATOM | 4237 | 0 | ALA | 63 | 21.006 | | 38.473 | | |
| ATOM | 4238 | N | PHE | 64 | 20.525 | 15.225 | 40.672 | 1.00 23.91 | CPS5 |
| ATOM | 4239 | CA | PHE | 64 | 20.591 | 13.782 | 40.916 | 1.00 25.22 | CPS5 |
| MOTA | 4240 | CB | PHE | 64 | 20.463 | 13.512 | 42.419 | 1.00 24.79 | CPS5 |
| MOTA | 4241 | CG | PHE | 64 | 20.781 | 12.097 | 42.818 | 1.00 27.22 | CPS5 |
| ATOM | 4242 | CD1 | PHE | 64 | 22.094 | 11.642 | 42.822 | 1.00 28.51 | CPS5 |
| ATOM | 4243 | CD2 | PHE | 64 | 19.768 | 11.233 | 43.217 | 1.00 27.62 | CPS5 |
| ATOM | 4244 | CE1 | PHE | 64 | 22.398 | 10.343 | 43.224 | 1.00 30.62 | CPS5 |
| ATOM | 4245 | CE2 | PHE | 64 | 20.061 | 9.931 | 43.622 | 1.00 28.83 | CPS5 |
| ATOM | 4246 | CZ | PHE | 64 | 21.377 | 9.489 | 43.625 | 1.00 28.53 | CPS5 |
| MOTA | 4247 | C | PHE | 64 | 19.453 | 13.109 | 40.147 | 1.00 26.39 | CPS5 |
| ATOM | 4248 | ō | PHE | 64 | 19.554 | 11.941 | 39.766 | 1.00 28.07 | CPS5 |
| ATOM | 4249 | N | GLY | 65 | 18.381 | 13.862 | 39.911 | 1.00 26.10 | CPS5 |
| | 4250 | CA | GLY | 65 | 17.251 | 13.368 | 39.143 | 1.00 27.17 | CPS5 |
| ATOM | | | | | | | | 1.00 28.46 | CPS5 |
| ATOM | 4251 | C | GLY | 65 | 16.088 | 12.768 | 39.905 | | CPS5 |
| ATOM | 4252 | 0 | GLY | 65 | 15.117 | 12.317 | 39.298 | 1.00 28.55 | |
| MOTA | 4253 | N | THR | 66 | 16.157 | 12.789 | 41.231 | 1.00 28.12 | CPS5 |
| MOTA | 4254 | CA | THR | 66 | 15.099 | 12.191 | 42.037 | 1.00 29.33 | CPS5 |
| MOTA | 4255 | CB | THR | 66 | 15.663 | 11.062 | 42.903 | 1.00 29.96 | CPS5 |
| MOTA | 4256 | OG1 | THR | 66 | 16.635 | 11.608 | 43.804 | 1.00 29.92 | CPS5 |
| ATOM | 4257 | CG2 | THR | 66 | 16.326 | 10.009 | 42.038 | 1.00 30.68 | CPS5 |
| ATOM | 4258 | C | THR | 66 | 14.410 | 13.148 | 42.984 | 1.00 28.71 | CPS5 |
| MOTA | 4259 | 0 | THR | 66 | 13.269 | 12.915 | 43.378 | 1.00 28.56 | CPS5 |
| MOTA | 4260 | N | GLY | 67 | 15.098 | 14.227 | 43.343 | 1.00 27.58 | CPS5 |
| ATOM | 4261 | CA | GLY | 67 | 14.530 | 15.150 | 44.305 | 1.00 27.06 | CPS5 |
| ATOM | 4262 | C | GLY | 67 | 14.741 | 14.479 | 45.657 | 1.00 27.43 | CPS5 |
| ATOM | 4263 | ō | GLY | 67 | 15.278 | 13.367 | 45.712 | 1.00 26.28 | CPS5 |
| | | N | ILE | 68 | 14.343 | 15.145 | 46.737 | 1.00 26.71 | CPS5 |
| ATOM | 4264 | | | | | | 48.082 | 1.00 28.68 | CPS5 |
| MOTA | 4265 | CA | ILE | 68 | 14.491 | 14.593 | | | |
| MOTA | 4266 | CB | ILE | 68 | 14.470 | 15.715 | 49.166 | 1.00 27.25 | CPS5 |
| ATOM | 4267 | | ILE | 68 | 14.574 | 15.098 | 50.569 | 1.00 27.25 | CPS5 |
| MOTA | 4268 | | ILE | 68 | 15.630 | 16.697 | 48.936 | 1.00 24.63 | CPS5 |
| MOTA | 4269 | CD1 | ILE | 68 | 17.030 | 16.084 | 49.112 | 1.00 23.40 | CPS5 |
| MOTA | 4270 | С | ILE | 68 | 13.335 | 13.629 | 48.342 | 1.00 30.86 | CPS5 |
| MOTA | 4271 | 0 | ILE | 68 | 12.167 | 13.982 | 48.169 | 1.00 31.01 | CPS5 |
| ATOM | 4272 | N | GLY | 69 | 13.671 | 12.412 | 48.752 | 1.00 33.01 | CPS5 |
| ATOM | 4273 | CA | GLY | 69 | 12.654 | 11.415 | 49.022 | 1.00 34.73 | CPS5 |
| ATOM | 4274 | C | GLY | 69 | 13.291 | 10.115 | 49.470 | 1.00 36.57 | CPS5 |
| 221011 | /3 | - | | | | | | | |

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| ATOM | 4275 | 0 | GLY | 69 | 14.363 | 10.112 | 50.079 | 1.00 36.27 | CPS5 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| ATOM | 4276 | N | ARG | 70 | 12.653 | 8.997 | 49.152 | 1.00 38.18 | CPS5 |
| ATOM | 4277 | CA | ARG | 70 | 13.203 | 7.724 | 49.579 | 1.00 39.66 | CPS5 |
| ATOM | 4278 | CB | ARG | 70 | 12.137 | 6.627 | 49.493 | 1.00 43.12 | CPS5 |
| MOTA | 4279 | CG | ARG | 70 | 11.182 | 6.661 | 50.696 | 1.00 47.23 | CPS5 |
| MOTA | 4280 | CD | ARG | 70 | 11.972 | 6.780 | 52.019 | 1.00 49.65 | CPS5 |
| ATOM | 4281 | NE | ARG | 70 | 11.469 | 7.858 | 52.870 | 1.00 51.86 | CPS5 |
| ATOM | 4282 | CZ | ARG | 70 | 12.239 | 8.672 | 53.590 | 1.00 52.77 | CPS5 |
| ATOM | 4283 | NH1 | | 70 | 13.558 | 8.540 | 53.569 | 1.00 53.05 | CPS5 |
| ATOM | 4284 | NH2 | | 70 | 11.691 | 9.627 | 54.328 | 1.00 52.96 | CPS5 |
| ATOM | 4285 | C | ARG | 70 | 14.468 | 7.317 | 48.855 | 1.00 37.80 | CPS5 |
| MOTA | 4286 | 0 | ARG | 70 | 15.221 | 6.478 | 49.345 | 1.00 37.07 | CPS5 |
| ATOM | 4287 | N | GLN | 71 | 14.726 | 7.926 | 47.703 | 1.00 36.29 | CPS5 |
| ATOM | 4288 | CA | GLN | 71 | 15.932 | 7.598 | 46.959 | 1.00 35.22 | CPS5 |
| ATOM | 4289 | CB | GLN | 71 | 15.707 | 7.778 | 45.453 | 1.00 36.48 | CPS5 |
| ATOM | 4290 | CG | GLN | 71 | 14.534 | 6.985 | 44.889 | 1.00 38.95 | CPS5 |
| ATOM | 4291 | CD | GLN | 71 | 14.402 | 7.129 | 43.379 | 1.00 40.20 | CPS5 |
| ATOM | 4292 | OE1 | | 71 | 15.236 | 6,631 | 42.622 | 1.00 40.67 | CPS5 |
| MOTA | 4293 | NE2 | | 71 | 13.355 | 7.827 | 42.937 | 1.00 40.72 | CPS5 |
| ATOM | 4294 | C | GLN | 71 | 17.084 | 8.483 | 47.412 | 1.00 33.38 | CPS5 |
| ATOM | 4295 | ō | GLN | 71 | 18.248 | 8.110 | 47.276 | 1.00 33.43 | CPS5 |
| ATOM | 4296 | N | LEU | 72 | 16.759 | 9.650 | 47.966 | 1,00 30.70 | CPS5 |
| ATOM | 4297 | CA | LEU | 72 | 17.786 | 10.591 | 48.409 | 1.00 27.96 | CPS5 |
| ATOM | 4298 | CB | LEU | 72 | 18.204 | 11.478 | 47.231 | 1.00 26.31 | CPS5 |
| ATOM | 4299 | CG | LEU | 72 | 19.285 | 12.532 | 47.448 | 1.00 26.21 | CPS5 |
| ATOM | 4300 | | LEU | 72 | 20.626 | 11.867 | 47.673 | 1.00 27.19 | CPS5 |
| ATOM | 4301 | | LEU | 72 | 19.338 | 13.446 | 46.213 | 1.00 25.53 | CPS5 |
| ATOM | 4302 | C | LEU | 72 | 17.279 | 11.469 | 49.556 | 1.00 27.62 | CPS5 |
| ATOM | 4303 | ō | LEU | 72 | 16.203 | 12.070 | 49.470 | 1.00 27.05 | CPS5 |
| ATOM | 4304 | N | SER | 73 | 18.076 | 11.545 | 50.616 | 1.00 26.31 | CPS5 |
| MOTA | 4305 | CA | SER | 73 | 17.735 | 12.323 | 51.805 | 1.00 25.42 | CPS5 |
| ATOM | 4306 | CB | SER | 73 | 17.889 | 11.441 | 53.051 | 1.00 26.75 | CPS5 |
| ATOM | 4307 | OG | SER | 73 | 17.970 | 12.228 | 54.231 | 1.00 27.96 | CPS5 |
| ATOM | 4308 | C | SER | 73 | 18.633 | 13.539 | 51.965 | 1.00 24.08 | CPS5 |
| ATOM | 4309 | ō | SER | 73 | 19.733 | 13.581 | 51.419 | 1.00 23.91 | CPS5 |
| MOTA | 4310 | N | PHE | 74 | 18.165 | 14.525 | 52.721 | 1.00 23.49 | CPS5 |
| ATOM | 4311 | CA | PHE | 74 | 18.975 | 15.707 | 52.995 | 1.00 23.97 | CPS5 |
| ATOM | 4312 | CB | PHE | 74 | 18.246 | 16.657 | 53.955 | 1.00 24.68 | CPS5 |
| ATOM | 4313 | CG | PHE | 74 | 17.124 | 17.430 | 53.319 | 1.00 25.48 | CPS5 |
| ATOM | 4314 | | PHE | 74 | 17.392 | 18.421 | 52.371 | 1.00 26.10 | CPS5 |
| ATOM | 4315 | | PHE | 74 | 15.801 | 17.176 | 53.672 | 1.00 26.28 | CPS5 |
| ATOM | 4316 | | PHE | 74 | 16.347 | 19.151 | 51.786 | 1.00 25.75 | CPS5 |
| MOTA | 4317 | CE2 | PHE | 74 | 14.750 | 17.896 | 53.092 | 1.00 26.75 | CPS5 |
| ATOM | 4318 | CZ | PHE | 74 | 15.028 | 18.886 | 52.148 | 1.00 25.31 | CPS5 |
| ATOM | 4319 | C | PHE | 74 | 20.260 | 15.241 | 53.674 | 1.00 23.42 | CPS5 |
| ATOM | 4320 | Ó | PHE | 74 | 21.334 | 15.804 | 53.459 | 1.00 23.30 | CPS5 |
| ATOM | 4321 | N | GLN | 75 | 20.141 | 14.207 | 54.504 | 1.00 24.48 | CPS5 |
| ATOM | 4322 | CA | GLN | 75 | 21.284 | 13.688 | 55.245 | 1.00 24.75 | CPS5 |
| MOTA | 4323 | CB | GLN | 75 | 20.804 | 12.774 | 56.382 | 1.00 24.94 | CPS5 |
| MOTA | 4324 | CG | GLN | 75 | 20.012 | 13.515 | 57.455 | 1.00 24.64 | CPS5 |
| ATOM | 4325 | CD | GLN | 75 | 20.838 | 14.550 | 58.200 | 1.00 24.25 | CPS5 |
| ATOM | 4326 | | GLN | 75 | 20.304 | 15.559 | 58.674 | 1.00 28.14 | CPS5 |
| ATOM | 4327 | | GLN | 75 | 22.141 | 14.308 | 58.319 | 1.00 22.66 | CPS5 |
| ATOM | 4328 | С | GLN | 75 | 22.316 | 12.958 | 54.390 | 1.00 26.96 | CPS5 |
| ATOM | 4329 | 0 | GLN | 75 | 23.423 | 12.684 | | 1.00 27.29 | CPS5 |
| MOTA | 4330 | N | ASP | 76 | 21.965 | 12.651 | | | CPS5 |
| ATOM | 4331 | CA | ASP | 76 | 22.906 | 11.976 | | _ | CPS5 |
| | | | | - | • - • | | | | |

| ATOM | 4332 | CB | ASP | 76 | 22.171 | 11.187 | 51.157 | 1.00 28.71 | CPS5 |
|------|------|-----|-----|------------|--------|------------------|------------------|--------------------------|--------------|
| MOTA | 4333 | CG | ASP | 76 | 21.422 | 10.002 | 51.695 | 1.00 30.19 | CPS5 |
| ATOM | 4334 | OD1 | ASP | 76 | 21.971 | 9.327 | 52.593 | 1.00 30.44 | CPS5 |
| MOTA | 4335 | OD2 | ASP | 76 | 20.296 | 9.733 | 51.211 | 1.00 30.21 | CPS5 |
| MOTA | 4336 | C | ASP | 76 | 23.787 | 13.007 | 51.552 | 1.00 29.00 | CPS5 |
| MOTA | 4337 | 0 | ASP | 76 | 24.738 | 12.652 | 50.856 | 1.00 30.49 | CPS5 |
| ATOM | 4338 | N | ILE | 77 | 23.472 | 14.284 | 51.743 | 1.00 28.00 | CPS5 |
| ATOM | 4339 | CA | ILE | 7 7 | 24.207 | 15.354 | 51.080 | 1.00 27.42 | CPS5 |
| ATOM | 4340 | CB | ILE | 7 7 | 23.251 | 16.214 | 50.213 | 1.00 25.93 | CPS5 |
| ATOM | 4341 | CG2 | ILE | 7 7 | 24.067 | 17.152 | 49.328 | 1.00 26.70 | CPS5 |
| ATOM | 4342 | CG1 | ILE | 77 | 22.345 | 15.310 | 49.370 | 1.00 24.69 | CPS5 |
| MOTA | 4343 | CD1 | ILE | 7 7 | 21.036 | 15.971 | 48.941 | 1.00 25.15 | CPS5 |
| MOTA | 4344 | C | ILE | 77 | 24.910 | 16.287 | 52.046 | 1.00 28.47 | CPS5 |
| ATOM | 4345 | 0 | ILE | 77 | 24.287 | 16.853 | 52.943 | 1.00 29.75 | CPS5 |
| ATOM | 4346 | N | GLU | 78 | 26.206 | 16.472 | 51.864 | 1.00 27.86 | CPS5 |
| ATOM | 4347 | CA | GLU | 78 | 26.920 | 17.367 | 52.751 | 1.00 31.23 | CPS5 |
| ATOM | 4348 | CB | GLU | 78 | 27.892 | 16.591 | 53.638 | 1.00 32.64 | CPS5 |
| MOTA | 4349 | CG | GLU | 78 | 28.558 | 17.466 | 54.681 | 1.00 34.90 | CPS5 |
| MOTA | 4350 | CD | GLU | 78 | 29.270 | 16.647 | 55.734 | 1.00 37.57 | CPS5 |
| ATOM | 4351 | OE1 | GLU | 78 ' | 30.334 | 16.072 | 55.425 | 1.00 38.97 | CPS5 |
| ATOM | 4352 | OE2 | GLU | 78 | 28.753 | 16.568 | 56.866 | 1.00 38.56 | CPS5 |
| ATOM | 4353 | C | GLU | 78 | 27.676 | 18.468 | 52.042 | 1.00 31.73 | CPS5 |
| ATOM | 4354 | 0 | GLU | 78 | 28.415 | 18.224 | 51.090 | 1.00 32.74 | CPS5 |
| MOTA | 4355 | N | ILE | 79 | 27.481 | 19.691 | 52.508 | 1.00 32.96 | CPS5 |
| MOTA | 4356 | CA | ILE | 79 | 28.177 | 20.821 | 51.932 | 1.00 35.99 | CPS5 |
| MOTA | 4357 | CB | ILE | 79 | 27.265 | 22.044 | 51.818 | 1.00 36.51 | CPS5 |
| ATOM | 4358 | CG2 | ILE | 79 | 28.066 | 23.252 | 51.363 | 1.00 35.93 | CPS5 |
| ATOM | 4359 | CG1 | ILE | 79 | 26.129 | 21.738 | 50.842 | 1.00 37.54 | CPS5 |
| MOTA | 4360 | CD1 | ILE | 79 | 25.122 | 22.836 | 50.754 | 1.00 42.06 | CPS5 |
| ATOM | 4361 | C | ILE | 79 | 29.342 | 21.145 | 52.842 | 1.00 38.38 | CPS5 |
| MOTA | 4362 | 0 | ILE | 79 | 29.166 | 21.432 | 54.026 | 1.00 37.01 | CPS5 |
| MOTA | 4363 | N | ARG | 80 | 30.543 | 21.075 | 52.290 | 1.00 42.32 | CPS5 |
| MOTA | 4364 | CA | ARG | 80 | 31.729 | 21.371 | 53.070 | 1.00 46.50 | CPS5 |
| MOTA | 4365 | CB | ARG | 80 | 32.690 | 20.180 | 53.091 | 1.00 46.70 | CPS5 |
| MOTA | 4366 | CG | ARG | 80 | 32.116 | 18.913 | 53.670 | 1.00 48.52 | CPS5 |
| MOTA | 4367 | CD | ARG | 80 | 33.151 | 17.798 | 53.687 | 1.00 49.02 | CPS5 |
| MOTA | 4368 | NE | ARG | 80 | 32.519 | 16.508 | 53.945 | 1.00 50.86 | CPS5 |
| MOTA | 4369 | CZ | ARG | 80 | 33.159 | 15.345 | 53.970 | 1.00 50.68 | CPS5 |
| MOTA | 4370 | | ARG | 80 | 34.465 | 15.303 | 53.757 | 1.00 50.94 | CPS5 |
| MOTA | 4371 | | ARG | 80 | 32.485 | 14.221 | 54.185 | 1.00 51.63 | CPS5 CPS5 |
| MOTA | 4372 | C | ARG | 80 | 32,444 | 22.545 | 52.459 | 1.00 48.41 | CPS5 |
| MOTA | 4373 | 0 | ARG | 80 | 31.955 | 23.189 | 51.529 | 1.00 48.48 | CPS5 |
| MOTA | 4374 | N | LYS | 81 | 33.616 | 22.820 | 53.003 | 1.00 51.83 1.00 54.26 | CPS5 |
| MOTA | 4375 | CA | LYS | 81 | 34.448 | 23.892 | 52.507 | 1.00 55.70 | CPS5 |
| ATOM | 4376 | CB | LYS | 81 | 34.388 | 25.099 | 53.445 | 1.00 58.10 | CPS5 |
| ATOM | 4377 | CG | LYS | 81 | 32.994 | 25.704 | 53.578 | 1.00 59.69 | CPS5 |
| ATOM | 4378 | CD | LYS | 81 | 33.014 | 26.958 | 54.439 | 1.00 61.09 | CPS5 |
| MOTA | 4379 | CE | LYS | 81 | 31.606 | 27.467 | 54.730 | 1.00 61.03 | CPS5 |
| ATOM | 4380 | NZ | LYS | 81 | 30.801 | 26.502 | 55.540 | | CPS5 |
| MOTA | 4381 | C | LYS | 81 | 35.847 | 23.307 22.695 | 52.459 53.427 | | CPS5 |
| ATOM | 4382 | 0 | LYS | 81 | 36.305 | | 53.427 | | CPS5 |
| ATOM | 4383 | N | ASP | 82 | 36.504 | 23.452 | 51.314 | | CPS5 |
| ATOM | 4384 | CA | ASP | 82 | 37.855 | 22.940 | | | CPS5 |
| ATOM | 4385 | CB | ASP | 82 | 38.281 | 23.026 | | | CPS5 |
| ATOM | 4386 | CG | ASP | 82 | 37.874 | 24.337 | | | CPS5 |
| MOTA | 4387 | | ASP | 82 | 37.980 | 25.399 | | | CPS5 |
| ATOM | 4388 | 002 | ASP | 82 | 37.457 | 24.301 | 41.003 | 1.00 37.30 | 0.00 |
| | | | | | | | | | |

| 7 more | 4300 | ~ | 7 C D | 0.0 | 20 010 | 00 750 | | | |
|--------|------|-------|-----------|-----|--------|--------|--------|------------|------|
| ATOM | 4389 | C | ASP | 82 | 38.810 | 23.753 | 52.015 | 1.00 57.41 | CPS5 |
| MOTA | 4390 | 0 | ASP | 82 | 38.377 | 24.523 | 52.874 | 1.00 56.93 | CPSS |
| MOTA | 4391 | И | GLN | 83 | 40.107 | 23.580 | 51.785 | 1.00 58.43 | CPS5 |
| MOTA | 4392 | CA | GLN | 83 | 41.119 | 24.306 | 52.543 | 1.00 59.77 | CPS5 |
| ATOM | 4393 | CB | GLN | 83 | 42.505 | 23.717 | 52.275 | 1.00 60.54 | CPS5 |
| ATOM | 4394 | CG | GLN | 83 | 42.754 | 22.364 | 52.916 | 1.00 61.21 | CPS5 |
| ATOM | 4395 | CD | GLN | 83 | 42.737 | 22.424 | 54.432 | 1.00 61.78 | CPS5 |
| ATOM | 4396 | OE1 | GLN | 83 | 41.674 | 22.447 | 55.054 | 1.00 62.24 | CPS5 |
| ATOM | 4397 | NE2 | GLN | 83 | 43.921 | 22.462 | 55.035 | 1.00 61.85 | CPS5 |
| ATOM | 4398 | C | GLN | 83 | 41.117 | 25.793 | 52.189 | 1.00 60.23 | CPS5 |
| ATOM | 4399 | 0 | GLN | 83 | 41.792 | 26.598 | 52.837 | 1.00 60.80 | CPS5 |
| ATOM | 4400 | N | ASN | 84 | 40.359 | 26.153 | 51.157 | 1.00 59.89 | CPS5 |
| ATOM | 4401 | CA | ASN | 84 | 40.268 | 27.543 | 50.730 | 1.00 59.63 | CPS5 |
| ATOM | 4402 | CB | ASN | 84 | 40.373 | 27.636 | 49.207 | 1.00 60.60 | |
| ATOM | 4402 | CG | ASN | | | | | | CPS5 |
| | | | | 84 | 41.707 | 27.140 | 48.685 | 1.00 61.37 | CPS5 |
| MOTA | 4404 | | ASN | 84 | 42.761 | 27.667 | 49.044 | 1.00 61.62 | CPS5 |
| ATOM | 4405 | | ASN | 84 | 41.669 | 26.120 | 47.834 | 1.00 61.98 | CPS5 |
| MOTA | 4406 | C | ASN | 84 | 38.956 | 28.160 | 51.199 | 1.00 59.10 | CPS5 |
| MOTA | 4407 | 0 | ASN | 84 | 38.731 | 29.361 | 51.037 | 1.00 59.66 | CPS5 |
| MOTA | 4408 | N | GLY | 85 | 38.095 | 27.330 | 51.780 | 1.00 57.75 | CPS5 |
| ATOM | 4409 | CA | GLY | 85 | 36.818 | 27.809 | 52.272 | 1.00 56.41 | CPS5 |
| ATOM | 4410 | C | GLY | 85 | 35.731 | 27.794 | 51.213 | 1.00 55.75 | CPS5 |
| ATOM | 4411 | 0 | GLY | 85 | 34.643 | 28.331 | 51.425 | 1.00 56.16 | CPS5 |
| ATOM | 4412 | N | LYS | 86 | 36.022 | 27.180 | 50.070 | 1.00 54.26 | CPS5 |
| ATOM | 4413 | CA | LYS | 86 | 35.058 | 27.107 | 48.978 | 1.00 52.12 | CPS5 |
| ATOM | 4414 | CB | LYS | 86 | 35.775 | 26.812 | 47.657 | 1.00 53.72 | CPS5 |
| ATOM | 4415 | CG | LYS | 86 | 34.948 | 27.105 | 46.406 | 1.00 55.30 | CPS5 |
| ATOM | 4416 | CD | LYS | 86 | 34.812 | 28.604 | 46.171 | 1.00 56.46 | CPS5 |
| MOTA | 4417 | CE | LYS | 86 | 34.012 | 28.910 | 44.905 | 1.00 56.79 | CPS5 |
| MOTA | 4418 | NZ | LYS | 86 | 32.619 | 28.397 | 45.007 | 1.00 57.01 | CPS5 |
| MOTA | 4419 | С | LYS | 86 | 34.057 | 25.999 | 49.279 | 1.00 49.78 | CPS5 |
| MOTA | 4420 | 0 | LYS | 86 | 34.420 | 24.944 | 49.806 | 1.00 49.58 | CPS5 |
| MOTA | 4421 | N | PRO | 87 | 32.777 | 26.222 | 48.952 | 1.00 47.09 | CPS5 |
| MOTA | 4422 | CD | PRO | 87 | 32.162 | 27.432 | 48.380 | 1.00 46.07 | CPS5 |
| MOTA | 4423 | CA | PRO | 87 | 31.764 | 25.198 | 49.214 | 1.00 44.34 | CPS5 |
| ATOM | 4424 | CB | PRO | 87 | 30.469 | 25.995 | 49.177 | 1.00 44.60 | CPS5 |
| ATOM | 4425 | CG | PRO | 87 | 30.745 | 26.967 | 48.074 | 1.00 45.82 | CPS5 |
| ATOM | 4426 | C | PRO | 87 | 31.776 | 24.098 | 48.158 | 1.00 40.83 | CPS5 |
| ATOM | 4427 | 0 | PRO | 87 | 31.837 | 24.382 | 46.961 | 1.00 40.94 | CPS5 |
| ATOM | 4428 | N | TYR | 88 | 31.731 | 22.846 | 48.598 | 1.00 37.82 | CPS5 |
| ATOM | 4429 | CA | TYR | 88 | 31.690 | 21.737 | 47.662 | 1.00 34.81 | CPS5 |
| ATOM | 4430 | CB | TYR | 88 | 33.111 | 21.229 | 47.335 | 1.00 35.73 | CPS5 |
| MOTA | 4431 | CG | TYR | 88 | 33.795 | 20.385 | 48.390 | 1.00 34.31 | CPS5 |
| MOTA | 4432 | CD1 | TYR | 88 | 33.648 | 19.002 | 48.399 | 1.00 34.27 | CPS5 |
| MOTA | 4433 | | TYR | 88 | 34.303 | 18.212 | 49.339 | 1.00 34.82 | CPS5 |
| ATOM | 4434 | | TYR | 88 | 34.615 | 20.966 | 49.354 | 1.00 35.40 | CPS5 |
| ATOM | 4435 | | TYR | 88 | 35.275 | 20.187 | 50.304 | 1.00 33.64 | CPS5 |
| ATOM | 4436 | CZ | TYR | 88 | 35.112 | 18.812 | 50.290 | 1.00 35.08 | CPS5 |
| ATOM | 4437 | OH | TYR | 88 | 35.730 | 18.028 | 51.239 | 1.00 35.18 | CPS5 |
| ATOM | 4438 | C | TYR | 88 | 30.807 | 20.668 | 48.279 | 1.00 33.39 | CPS5 |
| ATOM | 4439 | ō | TYR | 88 | 30.627 | 20.633 | 49.497 | 1.00 32.83 | CPS5 |
| ATOM | 4440 | N | ILE | 89 | 30.238 | 19.817 | 47.435 | 1.00 31.13 | CPS5 |
| ATOM | 4441 | CA | ILE | 89 | 29.321 | 18.778 | 47.882 | 1.00 30.93 | CPS5 |
| ATOM | 4442 | CB | ILE | 89 | 28.043 | 18.780 | 47.010 | 1.00 29.10 | CPS5 |
| ATOM | 4443 | | ILE | 89 | 27.189 | 17.547 | 47.303 | 1.00 27.98 | CPS5 |
| ATOM | 4444 | | ILE | 89 | 27.253 | 20.065 | 47.253 | 1.00 27.68 | CPS5 |
| ATOM | 4445 | | ILE | 89 | 26.041 | 20.215 | 46.364 | 1.00 27.97 | CPS5 |
| ALON | | بدسيب | يند سي حد | رد | 20.041 | 40.213 | .0.504 | , | |

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| ATOM | 4446 | C | ILE | 89 | 29.873 | 17.362 | 47.863 | 1.00 32.51 | CPS5 |
|------|------|-----|-----|----------|--------|--------|--------|------------|------|
| ATOM | 4447 | 0 | ILE | 89 | 30.637 | 16.987 | 46.973 | 1.00 31.03 | CPS5 |
| ATOM | 4448 | N | ILE | 90 | 29.462 | 16.582 | 48.858 | 1.00 33.80 | CPS5 |
| MOTA | 4449 | CA | ILE | 90 | 29.837 | 15.180 | 48.960 | | |
| | | | | | | | | 1.00 35.56 | CPS5 |
| ATOM | 4450 | CB | ILE | 90 | 30.776 | 14.928 | 50.144 | 1.00 37.43 | CPS5 |
| ATOM | 4451 | CG2 | | 90 | 30.959 | 13.418 | 50.359 | 1.00 37.12 | CPS5 |
| ATOM | 4452 | | ILE | 90 | 32.116 | 15.608 | 49.875 | 1.00 38.91 | CPS5 |
| ATOM | 4453 | CD1 | | 90 | 33.093 | 15.508 | 51.006 | 1.00 42.45 | CPS5 |
| MOTA | 4454 | C | ILE | 90 | 28.564 | 14.363 | 49.156 | 1.00 36.47 | CPS5 |
| ATOM | 4455 | 0 | ILE | 90 | 27.782 | 14.624 | 50.076 | 1.00 35.64 | CPS5 |
| MOTA | 4456 | N | CYS | 91 | 28.348 | 13.400 | 48.269 | 1.00 36.91 | CPS5 |
| MOTA | 4457 | CA | CYS | 91 | 27.189 | 12.520 | 48.340 | 1.00 40.22 | CPS5 |
| ATOM | 4458 | CB | CYS | 91 | 26.132 | 12.945 | 47.328 | 1.00 37.91 | CPS5 |
| ATOM | 4459 | SG | CYS | 91 | 24.623 | 11.970 | 47.401 | 1.00 39.23 | CPS5 |
| ATOM | 4460 | С | CYS | 91 | 27.643 | 11.094 | 48.035 | 1.00 42.93 | CPS5 |
| ATOM | 4461 | ō | CYS | 91 | 27.983 | 10.771 | 46.895 | 1.00 42.83 | CPS5 |
| ATOM | 4462 | N | THR | 92 | 27.648 | 10.245 | 49.056 | 1.00 46.74 | CPS5 |
| ATOM | 4463 | CA | THR | 92 | 28.070 | 8.858 | 48.881 | 1.00 50.26 | CPS5 |
| ATOM | 4464 | CB | THR | 92 | 28.080 | 8.106 | 50.238 | 1.00 51.61 | CPS5 |
| ATOM | 4465 | OG1 | | 92 | 28.496 | 6.748 | 50.035 | 1.00 52.93 | CPS5 |
| ATOM | 4466 | CG2 | THR | 92 | 26.693 | 8.130 | 50.876 | 1.00 52.55 | CPS5 |
| | | | | | | | | | CPS5 |
| ATOM | 4467 | C | THR | 92 | 27.175 | 8.110 | 47.890 | 1.00 51.62 | |
| ATOM | 4468 | 0 | THR | 92 | 27.656 | 7.285 | 47.108 | 1.00 51.98 | CPS5 |
| MOTA | 4469 | N | LYS | 93 | 25.879 | 8.413 | 47.914 | 1.00 52.57 | CPS5 |
| ATOM | 4470 | CA | LYS | 93 | 24.918 | 7.769 | 47.020 | 1.00 53.74 | CPS5 |
| ATOM | 4471 | CB | LYS | 93 | 23.503 | 8.289 | 47.296 | 1.00 54.52 | CPS5 |
| ATOM | 4472 | CG | LYS | 93 | 23.041 | 8.147 | 48.742 | 1.00 56.49 | CPS5 |
| ATOM | 4473 | CD | LYS | 93 | 22.706 | 6.708 | 49.101 | 1.00 57.62 | CPS5 |
| MOTA | 4474 | CE | LYS | 93 | 21.372 | 6.279 | 48.501 | 1.00 58.57 | CPS5 |
| MOTA | 4475 | NZ | LYS | 93 | 20.218 | 7.009 | 49.109 | 1.00 59.31 | CPS5 |
| MOTA | 4476 | C | LYS | 93 | 25.262 | 8.027 | 45.556 | 1.00 53.90 | CPS5 |
| ATOM | 4477 | 0 | LYS | 93 | 24.681 | 7.419 | 44.656 | 1.00 54.01 | CPS5 |
| ATOM | 4478 | И | LEU | 94 | 26.213 | 8.926 | 45.322 | 1.00 53.85 | CPS5 |
| ATOM | 4479 | CA | LEU | 94 | 26.605 | 9.283 | 43.967 | 1.00 54.05 | CPS5 |
| MOTA | 4480 | CB | LEU | 94 | 26.967 | 10.770 | 43.904 | 1.00 54.55 | CPS5 |
| MOTA | 4481 | CG | LEU | 94 | 26.620 | 11.562 | 42.640 | 1.00 54.80 | CPS5 |
| ATOM | 4482 | CD1 | LEU | 94 | 27.225 | 12.951 | 42.751 | 1.00 54.69 | CPS5 |
| ATOM | 4483 | CD2 | LEU | 94 | 27.143 | 10.857 | 41.405 | 1.00 55.41 | CPS5 |
| ATOM | 4484 | C | LEU | 94 | 27.780 | 8.466 | 43.452 | 1.00 54.05 | CPS5 |
| ATOM | 4485 | 0 | LEU | 94 | 28.797 | 8.322 | 44.130 | 1.00 54.64 | CPS5 |
| ATOM | 4486 | N | SER | 95 | 27.626 | 7.934 | 42.246 | 1.00 53.47 | CPS5 |
| MOTA | 4487 | CA | SER | 95 | 28.673 | 7.155 | 41.603 | 1.00 53.51 | CPS5 |
| ATOM | 4488 | CB | SER | 95 | 28.131 | 6.559 | 40.299 | 1.00 54.31 | CPS5 |
| ATOM | 4489 | OG | SER | 95 | 29.138 | 5.881 | 39.574 | 1.00 56.70 | CPS5 |
| ATOM | 4490 | C | SER | 95 | 29.812 | 8.134 | 41.315 | 1.00 52.59 | CPS5 |
| ATOM | 4491 | o | SER | 95 | 29.589 | 9.345 | 41.279 | 1.00 53.14 | CPS5 |
| ATOM | 4492 | N | PRO | 96 | 31.046 | 7.636 | 41.121 | 1.00 51.05 | CPS5 |
| | 4493 | CD | PRO | 96 | 31.511 | 6.248 | 40.992 | 1.00 51.64 | CPS5 |
| MOTA | | | PRO | | 32.140 | 8.572 | 40.843 | 1.00 49.02 | CPS5 |
| MOTA | 4494 | CA | | 96 06 | | | | 1.00 50.01 | CPS5 |
| ATOM | 4495 | CB | PRO | 96 | 33.252 | 7.670 | 40.285 | 1.00 50.01 | CPS5 |
| ATOM | 4496 | CG | PRO | 96 | 32.537 | 6.387 | 39.898 | 1.00 31.26 | CPS5 |
| ATOM | 4497 | C | PRO | 96 | 31.731 | 9.680 | 39.878 | | CPS5 |
| ATOM | 4498 | 0 | PRO | 96 | 31.238 | 9.425 | 38.775 | 1.00 46.21 | |
| MOTA | 4499 | N | ALA | 97 | 31.931 | 10.917 | 40.313 | 1.00 44.30 | CPS5 |
| MOTA | 4500 | CA | ALA | 97 | 31.566 | 12.063 | 39.499 | 1.00 41.77 | CPS5 |
| ATOM | 4501 | CB | ALA | 97 | 30.055 | 12.176 | 39.425 | 1.00 40.64 | CPS5 |
| ATOM | 4502 | C | ALA | 97 | 32.140 | 13.342 | 40.071 | 1.00 40.33 | CPS5 |
| | | | | | | | | | |

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| ATOM | 4503 | 0 | ALA | 97 | 32.593 | 13.382 | 41.216 | 1.00 40.58 | CPS5 |
|--------|------|-----|--------|-----|--------|--------|--------|------------|------|
| MOTA | 4504 | N | ALA | 98 | 32.121 | 14.387 | 39.256 | 1.00 37.31 | CPS5 |
| ATOM | 4505 | CA | ALA | 98 | 32.597 | 15.688 | 39.676 | 1.00 34.75 | CPS5 |
| ATOM | 4506 | CB | ALA | 98 | 33.398 | 16.340 | 38.561 | 1.00 35.64 | CPS5 |
| MOTA | 4507 | С | ALA | 98 | 31.308 | 16.463 | 39.941 | 1.00 32.51 | CPS5 |
| MOTA | 4508 | 0 | ALA | 98 | 30.407 | 16.478 | 39.107 | 1.00 31.77 | CPS5 |
| ATOM | 4509 | N | VAL | 99 | 31.204 | 17.061 | 41.119 | 1.00 29.38 | CPS5 |
| ATOM | 4510 | CA | VAL | 99 | 30.017 | 17.823 | 41.476 | 1.00 26.77 | CPS5 |
| MOTA | 4511 | CB | VAL | 99 | 29.409 | 17.320 | 42.808 | 1.00 26.38 | CPS5 |
| ATOM | 4512 | CG1 | VAL | 99 | 28.128 | 18.089 | 43.132 | 1.00 25.70 | CPS5 |
| ATOM | 4513 | CG2 | VAL | 99 | 29.110 | 15.821 | 42.708 | 1.00 26.03 | CPS5 |
| ATOM | 4514 | С | VAL | 99 | 30.460 | 19.270 | 41.632 | 1.00 25.29 | CPS5 |
| MOTA | 4515 | 0 | VAL | 99 | 31.518 | 19.541 | 42.192 | 1.00 24.54 | CPS5 |
| ATOM | 4516 | N | HIS | 100 | 29.655 | 20.190 | 41.113 | 1.00 23.97 | CPS5 |
| ATOM | 4517 | CA | HIS | 100 | 29.949 | 21.615 | 41.203 | 1.00 23.10 | CPS5 |
| ATOM | 4518 | CB | HIS | 100 | 30.225 | 22.176 | 39.819 | 1.00 24.86 | CPS5 |
| ATOM | 4519 | CG | HIS | 100 | 31.328 | 21.468 | 39.105 | 1.00 26.57 | CPS5 |
| ATOM | 4520 | CD2 | HIS | 100 | 31.297 | 20.480 | 38.181 | 1.00 27.57 | CPS5 |
| MOTA | 4521 | ND1 | HIS | 100 | 32.660 | 21.719 | 39.358 | 1.00 28.54 | CPS5 |
| ATOM | 4522 | | HIS | 100 | 33.403 | 20.915 | 38.618 | 1.00 28.60 | CPS5 |
| ATOM | 4523 | | HIS | 100 | 32.599 | 20.155 | 37.894 | 1.00 28.27 | CPS5 |
| ATOM | 4524 | C | HIS | 100 | 28.728 | 22.293 | 41.791 | 1.00 22.08 | CPS5 |
| ATOM | 4525 | 0 | HIS | 100 | 27.602 | 21.917 | 41.475 | 1.00 21.49 | CPS5 |
| ATOM | 4526 | N | VAL | 101 | 28.944 | 23.288 | 42.640 | 1.00 20.70 | CPS5 |
| MOTA | 4527 | CA | VAL | 101 | 27.823 | 23.980 | 43.254 | 1.00 20.32 | CPS5 |
| ATOM | 4528 | CB | VAL | 101 | 27.503 | 23.372 | 44.672 | 1.00 21.79 | CPS5 |
| ATOM | 4529 | CG1 | VAL | 101 | 28.687 | 23.560 | 45.614 | 1.00 21.73 | CPS5 |
| ATOM | 4530 | | VAL | 101 | 26.253 | 24.021 | 45.281 | 1.00 20.57 | CPS5 |
| ATOM | 4531 | С | VAL | 101 | 28.137 | 25.462 | 43.385 | 1.00 20.62 | CPS5 |
| ATOM | 4532 | 0 | VAL | 101 | 29.299 | 25.863 | 43.370 | 1.00 20.26 | CPS5 |
| MOTA | 4533 | N | SER | 102 | 27.091 | 26.281 | 43.448 | 1.00 18.85 | CPS5 |
| MOTA | 4534 | CA | SER | 102 | 27.256 | 27.709 | 43.670 | 1.00 18.73 | CPS5 |
| ATOM | 4535 | CB | SER | 102 | 27.292 | 28.509 | 42.363 | 1.00 19.66 | CPS5 |
| ATOM | 4536 | OG | SER | 102 | 27.474 | 29.886 | 42.685 | 1.00 19.70 | CPS5 |
| ATOM | 4537 | C | SER | 102 | 26.037 | 28.118 | 44.489 | 1.00 19.25 | CPS5 |
| MOTA | 4538 | 0 | SER | 102 | 24.931 | 27.684 | 44.200 | 1.00 17.98 | CPS5 |
| MOTA | 4539 | N | ILE | 103 | 26.246 | 28.928 | 45.520 | 1.00 19.07 | CPS5 |
| MOTA | 4540 | CA | ILE | 103 | 25.153 | 29.374 | 46.377 | 1.00 20.39 | CPS5 |
| ATOM | 4541 | CB | ILE | 103 | 25.347 | 28.876 | 47.833 | 1.00 22.16 | CPS5 |
| ATOM | 4542 | CG2 | | 103 | 24.216 | 29.404 | 48.736 | 1.00 22.36 | CPS5 |
| ATOM | 4543 | CG1 | | 103 | 25.363 | 27.350 | 47.865 | 1.00 21.89 | CPS5 |
| ATOM | 4544 | CD1 | ILE | 103 | 25.821 | 26.762 | 49.214 | 1.00 24.06 | CPS5 |
| MOTA | 4545 | С | ILE | 103 | 25.157 | 30.892 | 46.358 | 1.00 21.36 | CPS5 |
| MOTA | 4546 | 0 | ILE | 103 | 26.225 | 31.512 | 46.304 | 1.00 21.80 | CPS5 |
| ATOM | 4547 | N | THR | 104 | 23.968 | 31.489 | 46.374 | 1.00 21.34 | CPS5 |
| ATOM | 4548 | CA | THR | 104 | 23.839 | 32.938 | 46.347 | 1.00 22.25 | CPS5 |
| ATOM | 4549 | CB | THR | 104 | 23.591 | 33.450 | 44.901 | 1.00 24.00 | CPS5 |
| ATOM | 4550 | OG1 | | 104 | 23.661 | 34.887 | 44.864 | 1.00 24.60 | CPS5 |
| ATOM | 4551 | CG2 | | 104 | 22.235 | 32.998 | 44.399 | 1.00 23.88 | CPS5 |
| ATOM | 4552 | C | THR | 104 | 22.705 | 33.376 | 47.276 | 1.00 23.21 | CPS5 |
| ATOM | 4553 | o | THR | 104 | 21.831 | 32.579 | 47.641 | 1.00 21.95 | CPS5 |
| ATOM | 4554 | Ŋ | HIS | 105 | 22.728 | 34.645 | 47.664 | 1.00 24.23 | CPS5 |
| ATOM | 4555 | CA | HIS | 105 | 21.723 | 35.181 | 48.578 | 1.00 26.22 | CPS5 |
| ATOM | 4556 | CB | HIS | 105 | 22.287 | 35.276 | 50.003 | 1.00 27.67 | CPS5 |
| ATOM | 4557 | CG | HIS | 105 | 22.810 | 33.988 | 50.555 | 1.00 30.95 | CPS5 |
| ATOM | 4558 | | HIS | 105 | 24.036 | 33.417 | 50.475 | 1.00 32.56 | CPS5 |
| ATOM | 4559 | | HIS | 105 | 22.046 | 33.146 | 51.333 | 1.00 32.46 | CPS5 |
| , AION | 2,00 | | - 1113 | 100 | 22.040 | 55.110 | | | |
| | | | | | | | | | |

| MOTA | 4560 | | HIS | 105 | 22.777 | 32.114 | 51.713 | 1.00 32.44 | CPS5 |
|--------------|------|-----|-----|-----|------------------|--------|--------|------------|--------------|
| ATOM | 4561 | NE2 | HIS | 105 | 23.990 | 32.253 | 51.206 | 1.00 32.77 | CPS5 |
| MOTA | 4562 | C | HIS | 105 | 21.291 | 36.596 | 48.218 | 1.00 25.94 | CPS5 |
| ATOM | 4563 | 0 | HIS | 105 | 22.037 | 37.344 | 47.584 | 1.00 25.81 | CPS5 |
| ATOM | 4564 | N | THR | 106 | 20.077 | 36.944 | 48.630 | 1.00 25.98 | CPS5 |
| ATOM | 4565 | CA | THR | 106 | 19.569 | 38.305 | 48.498 | 1.00 26.59 | CPS5 |
| ATOM | 4566 | CB | THR | 106 | 18.474 | 38.498 | 47.436 | 1.00 26.91 | CPS5 |
| ATOM | 4567 | OG1 | THR | 106 | 17.305 | 37.771 | 47.813 | 1.00 26.20 | CPS5 |
| MOTA | 4568 | CG2 | THR | 105 | 18.963 | 38.070 | 46.062 | 1.00 25.16 | CPS5 |
| ATOM | 4569 | С | THR | 106 | 18.946 | 38.516 | 49.870 | 1.00 27.65 | CPS5 |
| ATOM | 4570 | 0 | THR | 106 | 19.024 | 37.638 | 50.733 | 1.00 26.71 | CPS5 |
| ATOM | 4571 | N | LYS | 107 | 18.330 | 39.667 | 50.086 | 1.00 28.18 | CPS5 |
| ATOM | 4572 | CA | LYS | 107 | 17.716 | 39.938 | 51.377 | 1.00 29.86 | CPS5 |
| ATOM | 4573 | СВ | LYS | 107 | 17.103 | 41.345 | 51.366 | 1.00 32.21 | CPS5 |
| ATOM | 4574 | CG | LYS | 107 | 16.495 | 41.791 | 52.690 | 1.00 36.65 | CPS5 |
| ATOM | 4575 | CD | LYS | 107 | 15.848 | 43.171 | 52.540 | 1.00 40.32 | CPS5 |
| MOTA | 4576 | CE | LYS | 107 | 15.282 | 43.682 | 53.860 | 1.00 42.28 | CPS5 |
| ATOM | 4577 | NZ | LYS | 107 | 14.641 | 45.026 | 53.709 | 1.00 45.02 | CPS5 |
| ATOM | 4578 | C | LYS | 107 | 16.645 | 38.910 | 51.754 | 1.00 29.02 | CPS5 |
| ATOM | 4579 | ō | LYS | 107 | 16.576 | 38.484 | 52.908 | 1.00 29.89 | CPS5 |
| ATOM | 4580 | И | GLU | 108 | 15.830 | 38.495 | 50.785 | 1.00 27.24 | CPS5 |
| MOTA | 4581 | CA | GLU | 108 | 14.733 | 37.568 | 51.063 | 1.00 26.97 | CPS5 |
| ATOM | 4582 | CB | GLU | 108 | 13.428 | 38.156 | 50.525 | 1.00 29.17 | CPS5 |
| ATOM | 4583 | CG | GLU | 108 | 13.129 | 39.552 | 51.030 | 1.00 35.90 | CPS5 |
| ATOM | 4584 | CD | GLU | 108 | 11.758 | 40.043 | 50.612 | 1.00 40.16 | CPS5 |
| ATOM | 4585 | OE1 | | 108 | 11.459 | 40.044 | 49.397 | 1.00 43.68 | CPS5 |
| MOTA | 4586 | OE2 | | 108 | 10.975 | 40.436 | 51.505 | 1.00 43.08 | CPS5 |
| ATOM | 4587 | C | GLU | 108 | 14.855 | 36.149 | 50.527 | 1.00 44.05 | CPS5 |
| ATOM | | 0 | GLU | 108 | 14.007 | 35.300 | 50.823 | 1.00 24.76 | CPS5 |
| ATOM | | И | TYR | 109 | 15.889 | 35.888 | 49.738 | 1.00 23.74 | CPS5 |
| ATOM | | CA | TYR | 109 | 16.045 | 34.564 | 49.137 | 1.00 23.02 | CPS5 |
| ATOM | | CB | TYR | 109 | 15.695 | 34.627 | 47.645 | 1.00 23.10 | CPS5 |
| ATOM | | CG | TYR | 109 | 14.286 | 35.052 | 47.352 | 1.00 23.49 | CPS5 |
| ATOM | | | TYR | 109 | 13.243 | 34.135 | 47.403 | 1.00 23.43 | CPS5 |
| ATOM | | CEI | | 109 | 11.931 | 34.529 | 47.199 | 1.00 24.25 | CPS5 |
| | | CD2 | | 109 | 13.982 | 36.390 | 47.133 | 1.00 24.00 | CPS5 |
| ATOM ATOM | | CE2 | | 109 | 12.667 | 36.797 | 46.874 | 1.00 25.20 | CPS5 |
| ATOM | | CZ | TYR | 109 | 11.648 | 35.861 | 46.937 | 1.00 25.55 | CPS5 |
| | | OH | TYR | 109 | 10.341 | 36.243 | 46.769 | 1.00 25.55 | CPS5 |
| ATOM | | C | TYR | 109 | | 33.976 | 49.230 | 1.00 20.33 | CPS5 |
| ATOM | | 0 | TYR | 109 | 17.438 18.421 | 34.691 | 49.403 | 1.00 22.03 | CPS5 |
| ATOM | | N | | | · · | 32.650 | 49.403 | 1.00 23.71 | CPS5 |
| ATOM | | | ALA | 110 | 17.490 | 31.912 | 49.126 | 1.00 21.41 | CPS5 |
| MOTA | | CA | ALA | 110 | 18.744 | | 50.258 | 1.00 20.41 | CPS5 |
| ATOM | | CB | ALA | 110 | 18.924 | 30.988 | 47.785 | 1.00 20.41 | CPS5 |
| ATOM | | C | ALA | 110 | 18.536 | 31.089 | | 1.00 20.71 | CPS5 |
| ATOM | | 0 | ALA | 110 | 17.415 | 30.635 | 47.508 | 1.00 21.39 | CPS5 |
| ATOM | | N | ALA | 111 | 19.589 | 30.915 | 46,991 | 1.00 19.32 | CPS5 |
| MOTA | | CA | ALA | 111 | 19.467 | 30.131 | 45.771 | | |
| ATOM | | CB | ALA | 111 | 19.215 | 31.033 | 44.575 | 1.00 18.98 | CPS5 CPS5 |
| ATOM | | C | ALA | 111 | 20.734 | 29.344 | 45.550 | 1.00 19.39 | CPS5 |
| ATOM | | 0 | ALA | 111 | 21.800 | 29.707 | 46.050 | 1.00 18.83 | |
| ATOM | | N | ALA | 112 | 20.623 | 28.269 | 44.786 | 1.00 18.45 | CPS5 |
| ATOM | | CA | ALA | 112 | 21.784 | 27.451 | 44.508 | 1.00 19.52 | CPS5 |
| ATOM | | CB | ALA | 112 | 22.008 | 26.481 | 45.655 | 1.00 19.65 | CPS5 |
| ATOM | | C | ALA | 112 | 21.617 | 26.679 | 43.212 | 1.00 18.81 | CPS5 |
| ATOM | | 0 | ALA | 112 | 20.502 | 26.442 | 42.764 | 1.00 17.20 | CPS5 |
| ATOM | 4616 | N | GLN | 113 | 22.733 | 26.311 | 42.599 | 1.00 19.37 | CPS5 |
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| MOTA | 4617 | CA | GLN | 113 | 22.663 | 25.499 | 41.400 | 1.00 20.01 | CPS5 |
|------|------|-----|-----|-----|--------|--------|--------|------------|------|
| MOTA | 4618 | CB | GLN | 113 | 22.890 | 26.321 | 40.135 | 1.00 23.47 | CPS5 |
| MOTA | 4619 | CG | GLN | 113 | 24.249 | 26.942 | 40.040 | 1.00 26.43 | CPS5 |
| MOTA | 4620 | CD | GLN | 113 | 24.463 | 27.640 | 38.705 | 1.00 30.41 | CPS5 |
| ATOM | 4621 | OE1 | GLN | 113 | 25.506 | 28.234 | 38.467 | 1.00 29.83 | CPS5 |
| ATOM | 4622 | NE2 | GLN | 113 | 23.466 | 27.567 | 37.831 | 1.00 33.75 | CPS5 |
| ATOM | 4623 | С | GLN | 113 | 23.735 | 24.439 | 41.518 | 1.00 19.96 | CPS5 |
| ATOM | 4624 | ō | GLN | 113 | 24.753 | 24.633 | 42.177 | 1.00 19.44 | CPS5 |
| ATOM | 4625 | N | VAL | 114 | 23.504 | 23.312 | 40.869 | | |
| | | | | | | | | 1.00 19.35 | CPS5 |
| ATOM | 4626 | CA | VAL | 114 | 24.462 | 22.221 | 40.924 | 1.00 19.11 | CPS5 |
| MOTA | 4627 | CB | VAL | 114 | 23.960 | 21.111 | 41.897 | 1.00 18.72 | CPS5 |
| MOTA | 4628 | | VAL | 114 | 24.791 | 19.828 | 41.721 | 1.00 20.30 | CPS5 |
| MOTA | 4629 | | VAL | 114 | 24.043 | 21.603 | 43.344 | 1.00 20.16 | CPS5 |
| ATOM | 4630 | C | VAL | 114 | 24.589 | 21.611 | 39.538 | 1.00 19.40 | CPS5 |
| MOTA | 4631 | 0 | VAL | 114 | 23.618 | 21.590 | 38.781 | 1.00 19.86 | CPS5 |
| MOTA | 4632 | N | VAL | 115 | 25.792 | 21.159 | 39.201 | 1.00 19.59 | CPS5 |
| MOTA | 4633 | CA | VAL | 115 | 26.017 | 20.436 | 37.956 | 1.00 19.26 | CPS5 |
| MOTA | 4634 | CB | VAL | 115 | 26.879 | 21.202 | 36.928 | 1.00 20.70 | CPS5 |
| MOTA | 4635 | CG1 | VAL | 115 | 27.182 | 20.280 | 35.725 | 1.00 19.97 | CPS5 |
| MOTA | 4636 | CG2 | LAV | 115 | 26.131 | 22.443 | 36.433 | 1.00 19.15 | CPS5 |
| ATOM | 4637 | С | VAL | 115 | 26.780 | 19.172 | 38.359 | 1.00 22.16 | CPS5 |
| ATOM | 4638 | 0 | VAL | 115 | 27.765 | 19.248 | 39.092 | 1.00 21.19 | CPS5 |
| ATOM | 4639 | N | ILE | 116 | 26.291 | 18.018 | 37.920 | 1.00 23.19 | CPS5 |
| ATOM | 4640 | CA | ILE | 116 | 26.965 | 16.749 | 38.201 | 1.00 25.23 | CPS5 |
| | | | | | | | 38.761 | 1.00 23.23 | CPS5 |
| ATOM | 4641 | CB | ILE | 116 | 25.983 | 15.681 | | | |
| ATOM | 4642 | | ILE | 116 | 26.717 | 14.347 | 38.952 | 1.00 24.03 | CPS5 |
| MOTA | 4643 | | ILE | 116 | 25.401 | 16.139 | 40.106 | 1.00 24.21 | CPS5 |
| ATOM | 4644 | CD1 | | 116 | 24.294 | 15.209 | 40.635 | 1.00 22.70 | CPS5 |
| MOTA | 4645 | C | ILE | 116 | 27.521 | 16.243 | 36.866 | 1.00 26.72 | CPS5 |
| MOTA | 4646 | 0 | ILE | 116 | 26.788 | 16.165 | 35.881 | 1.00 25.85 | CPS5 |
| MOTA | 4647 | N | GLU | 117 | 28.809 | 15.914 | 36.835 | 1.00 30.40 | CPS5 |
| MOTA | 4648 | CA | GLU | 117 | 29.447 | 15.401 | 35.615 | 1.00 35.53 | CPS5 |
| MOTA | 4649 | CB | GLU | 117 | 30.792 | 16.064 | 35.352 | 1.00 36.89 | CPS5 |
| MOTA | 4650 | CG | GLU | 117 | 30.816 | 17.554 | 35.274 | 1.00 39.07 | CPS5 |
| MOTA | 4651 | CD | GLU | 117 | 32.168 | 18.036 | 34.808 | 1.00 39.75 | CPS5 |
| ATOM | 4652 | OE1 | GLU | 117 | 32.457 | 17.877 | 33.605 | 1.00 40.89 | CPS5 |
| ATOM | 4653 | OE2 | GLU | 117 | 32.948 | 18.547 | 35.641 | 1.00 40.65 | CPS5 |
| ATOM | 4654 | C | GLU | 117 | 29.735 | 13.915 | 35.771 | 1.00 38.76 | CPS5 |
| ATOM | 4655 | 0 | GLU | 117 | 30.317 | 13.501 | 36.782 | 1.00 38.92 | CPS5 |
| ATOM | 4656 | N | ALA | 118 | 29.364 | 13.131 | 34.761 | 1.00 41.50 | CPS5 |
| ATOM | 4657 | CA | ALA | 118 | 29.596 | 11.689 | 34.784 | 1.00 44.75 | CPS5 |
| ATOM | 4658 | СВ | ALA | 118 | 29.047 | 11.049 | 33.508 | 1.00 45.12 | CPS5 |
| MOTA | 4659 | C | ALA | 118 | 31.095 | | | 1.00 46.14 | CPS5 |
| | | | | | 31.885 | 12.266 | 34.413 | 1.00 46.30 | CPS5 |
| MOTA | 4660 | | ALA | 118 | 31.460 | 10.367 | | | CPS5 |
| MOTA | 4661 | | | 118 | | | | 1.00 33.16 | CPS6 |
| ATOM | 4662 | С | GLY | 1 | 34.929 | 20.508 | 32.382 | | CPS6 |
| ATOM | 4663 | 0 | GLY | 1 | 35.455 | 21.500 | 31.885 | 1.00 34.15 | CPS6 |
| ATOM | 4664 | N | GLY | 1 | 36.363 | 18.424 | 32.401 | 1.00 38.41 | |
| ATOM | 4665 | CA | GLY | 1 | 35.171 | 19.118 | 31.815 | 1.00 34.91 | CPS6 |
| ATOM | 4666 | N | ILE | 2 | 34.133 | 20.587 | 33.435 | 1.00 30.97 | CPS6 |
| ATOM | 4667 | CA | ILE | 2 | 33.824 | 21.875 | 34.039 | | CPS6 |
| ATOM | 4668 | CB | ILE | 2 | 32.405 | 21.855 | 34.627 | 1.00 27.89 | CPS6 |
| ATOM | 4669 | CG2 | ILE | 2 | 32.168 | 23.101 | 35.474 | 1.00 27.12 | CPS6 |
| ATOM | 4670 | CG1 | ILE | 2 | 31.386 | 21.726 | 33.490 | 1.00 28.03 | CPS6 |
| ATOM | 4671 | | ILE | 2 | 29.965 | 21.432 | | 1.00 28.46 | CPS6 |
| ATOM | 4672 | C | ILE | 2 | 34.810 | | | | CPS6 |
| ATOM | 4673 | 0 | ILE | 2 | 35.117 | | | | CPS6 |
| | | - | | - | | | | | |

| ATOM | 4674 | N | TYR | 3 | 35.305 | 23.492 | 35.080 | 1.00 26.59 | CPS6 |
|------|------|-----|-------|----|--------|----------------|--------|------------|------|
| ATOM | 4675 | CA | TYR | 3 | 36.234 | 23.970 | 36.101 | 1.00 26.25 | CPS6 |
| ATOM | 4676 | CB | TYR | 3 | 37.102 | 25.091 | 35.540 | 1.00 27.53 | CPS6 |
| MOTA | 4677 | CG | TYR | 3 | 38.027 | 25.703 | 36.570 | 1.00 31.25 | CPS6 |
| MOTA | 4678 | CD1 | TYR | 3 | 39.171 | 25.027 | 36.999 | 1.00 32.43 | CPS6 |
| MOTA | 4679 | CE1 | TYR | 3 | 40.006 | 25.568 | 37.978 | 1.00 35.68 | CPS6 |
| ATOM | 4680 | CD2 | TYR | 3 | 37.738 | 26.937 | 37.146 | 1.00 31.55 | CPS6 |
| ATOM | 4681 | CE2 | TYR | 3 | 38.563 | 27.489 | 38.126 | 1.00 35.40 | CPS6 |
| ATOM | 4682 | CZ | TYR | 3 | 39.697 | 26.800 | 38.537 | 1.00 36.39 | CPS6 |
| MOTA | 4683 | OH | TYR | 3 | 40.525 | 27.355 | 39.488 | 1.00 39.51 | CPS6 |
| MOTA | 4684 | C | TYR | 3 | 35.451 | 24.482 | 37.316 | 1.00 25.81 | CPS6 |
| ATOM | 4685 | 0 | TYR | 3 | 35.762 | 24.145 | 38.469 | 1.00 24.16 | CPS6 |
| ATOM | 4686 | N | GLY | 4 | 34.437 | 25.301 | 37.058 | 1.00 22.42 | CPS6 |
| ATOM | 4687 | CA | GLY | 4 | 33.630 | 25.823 | 38.147 | 1.00 22.32 | CPS6 |
| MOTA | 4688 | C | GLY | 4 | 32.365 | 26.494 | 37.642 | 1.00 20.34 | CPS6 |
| ATOM | 4689 | 0 | GLY | 4 | 32.280 | 26.799 | 36.461 | 1.00 19.69 | CPS6 |
| MOTA | 4690 | N | ILE | 5 | 31.389 | 26.704 | 38.525 | 1.00 20.01 | CPS6 |
| MOTA | 4691 | CA | ILE | 5 | 30.140 | 27.366 | 38.143 | 1.00 20.35 | CPS6 |
| MOTA | 4692 | CB | ILE | 5 | 28.947 | 26.382 | 38.097 | 1.00 20.14 | CPS6 |
| ATOM | 4693 | CG2 | ILE | 5 | 29,291 | 25.224 | 37.159 | 1.00 19.26 | CPS6 |
| ATOM | 4694 | CG1 | ILE | 5 | 28.600 | 25.876 | 39.507 | 1.00 19.61 | CPS6 |
| ATOM | 4695 | CD1 | ILE | 5 | 27.418 | 24.871 | 39.535 | 1.00 21.63 | CPS6 |
| ATOM | 4696 | C | ILE | 5 | 29.832 | 28.481 | 39.119 | 1.00 20.43 | CPS6 |
| ATOM | 4697 | 0 | ILE | 5 | 30.337 | 28.505 | 40.242 | 1.00 20.18 | CPS6 |
| MOTA | 4698 | N | GLY | 6 | 29.009 | 29.426 | 38.686 | 1.00 19.58 | CPS6 |
| MOTA | 4699 | CA | GLY | 6 | 28.681 | 30.532 | 39.560 | 1.00 19.69 | CPS6 |
| ATOM | 4700 | C | GLY | 6 | 27.279 | 31.023 | 39.287 | 1.00 19.25 | CPS6 |
| ATOM | 4701 | 0 | GLY | 6 | 26.842 | 31.080 | 38.135 | 1.00 17.69 | CPS6 |
| ATOM | 4702 | N | LEU | 7 | 26.581 | 31.374 | 40.358 | 1.00 19.31 | CPS6 |
| ATOM | 4703 | CA | LEU | 7 | 25.214 | 31.865 | 40.262 | 1.00 20.65 | CPS6 |
| ATOM | 4704 | CB | LEU | 7 | 24.249 | 30.808 | 40.811 | 1.00 20.48 | CPS6 |
| MOTA | 4705 | CG | LEU | 7 | 22.781 | 31.222 | 40.967 | 1.00 21.08 | CPS6 |
| MOTA | 4706 | CDI | LEU | 7 | 22.175 | 31.455 | 39.576 | 1.00 22.40 | CPS6 |
| ATOM | 4707 | CD2 | LEU | 7 | 22.017 | 30.132 | 41.724 | 1.00 21.05 | CPS6 |
| ATOM | 4708 | C | LEU | 7 | 25.108 | 33.114 | 41.116 | 1.00 20.36 | CPS6 |
| ATOM | 4709 | 0 | LEU | 7 | 25.687 | 33.180 | 42.193 | 1.00 21.58 | CPS6 |
| ATOM | 4710 | N | ASP | 8 | 24.387 | 34.114 | 40.631 | 1.00 20.16 | CPS6 |
| ATOM | 4711 | CA | ASP | 8 | 24.188 | 35.310 | 41.423 | 1.00 21.86 | CPS6 |
| MOTA | 4712 | CB | ASP | 8 | 25.261 | 36.368 | 41.151 | 1.00 23.79 | CPS6 |
| MOTA | 4713 | CG | ASP | 8 | 25.018 | 37.637 | 41.948 | 1.00 26.23 | CPS6 |
| ATOM | 4714 | OD1 | ASP | 8 | 24.287 | 38.523 | 41.462 | 1.00 26.66 | CPS6 |
| ATOM | 4715 | OD2 | ASP | 8 | 25.523 | 37.725 | 43.081 | 1.00 27.19 | CPS6 |
| ATOM | 4716 | С | ASP | 8 | 22.838 | 35.93 5 | 41.173 | 1.00 21.30 | CPS6 |
| ATOM | 4717 | 0 | ASP | 8 | 22.379 | 35.977 | 40.041 | | CPS6 |
| MOTA | 4718 | N | ILE | 9 | 22.184 | 36.384 | 42.242 | | CPS6 |
| MOTA | 4719 | CA | ILE | 9 | 20.911 | 37.081 | 42.099 | 1.00 20.91 | CPS6 |
| MOTA | 4720 | CB | ILE | 9 | 19.733 | 36.347 | 42.787 | 1.00 21.99 | CPS6 |
| MOTA | 4721 | CG2 | ILE | 9 | 18.456 | 37.172 | 42.639 | 1.00 20.05 | CPS6 |
| ATOM | 4722 | CG | LILE | 9 | 19.543 | 34.963 | 42.159 | | CPS6 |
| MOTA | 4723 | CDI | LILE | 9 | 18.405 | 34.165 | 42.754 | | CPS6 |
| ATOM | 4724 | С | ILE | 9 | 21.160 | 38.402 | | | CPS6 |
| ATOM | 4725 | 0 | ILE | 9 | 21.683 | 38.420 | 43.918 | 1.00 23.20 | CPS6 |
| MOTA | 4726 | N | THR | 10 | 20.813 | 39.505 | 42.148 | 1.00 24.06 | CPS6 |
| MOTA | 4727 | CA | THR | 10 | 21.033 | 40.826 | 42.722 | | CPS6 |
| ATOM | 4728 | CB | THR | 10 | 22.125 | 41.578 | 41.915 | | CPS6 |
| ATOM | 4729 | OG: | L THR | 10 | 23.375 | 40.882 | 42.054 | | CPS6 |
| ATOM | 4730 | | 2 THR | 10 | 22.299 | 43.006 | 42.413 | 1.00 28.83 | CPS6 |
| | | | | | | | | | |

| ATOM | 4731 | С | THR | 10 | 19.734 | 41.626 | 42.734 | 1.00 25.30 | CPS6 |
|------|-------|-----|---------|----|--------|--------|--------|------------|------|
| MOTA | 4732 | 0 | THR | 10 | 18.978 | 41.620 | 41.762 | 1.00 24.09 | CPS6 |
| ATOM | 4733 | N | GLU | 11 | 19.475 | 42.290 | 43.857 | 1.00 24.60 | CPS6 |
| ATOM | 4734 | CA | GLU | 11 | 18.278 | 43.112 | 44.025 | 1.00 25.85 | |
| ATOM | 4735 | CB | GLU | 11 | 18.012 | | | | CPS6 |
| | | | | | | 43.306 | 45.525 | 1.00 26.85 | CPS6 |
| ATOM | 4736 | CG | GLU | 11 | 16.635 | 43.843 | 45.872 | 1.00 30.57 | CPS6 |
| ATOM | 4737 | CD | GLU | 11 | 16.506 | 44.224 | 47.342 | 1.00 33.54 | CPS6 |
| ATOM | 4738 | | GLU | 11 | 17.435 | 43.928 | 48.136 | 1.00 34.46 | CPS6 |
| ATOM | 4739 | OE2 | GLU | 11 | 15.469 | 44.821 | 47.701 | 1.00 34.21 | CPS6 |
| ATOM | 4740 | C | GLU | 11 | 18.533 | 44.467 | 43.354 | 1.00 25.21 | CPS6 |
| MOTA | 4741 | 0 | GLU | 11 | 19.499 | 45.150 | 43.694 | 1.00 26.16 | CPS6 |
| ATOM | 4742 | N | LEU | 12 | 17.687 | 44.855 | 42.402 | 1.00 26.01 | CPS6 |
| MOTA | 4743 | CA | LEU | 12 | 17.870 | 46.138 | 41.713 | 1.00 28.08 | CPS6 |
| ATOM | 4744 | CB | LEU | 12 | 16.733 | 46.381 | 40.707 | 1.00 28.52 | CPS6 |
| ATOM | 4745 | CG | LEU | 12 | 16.880 | 45.889 | 39.264 | 1.00 31.49 | CPS6 |
| ATOM | 4746 | | LEU | 12 | 17.467 | 44.495 | 39.234 | 1.00 30.71 | CPS6 |
| | | | | | | | | | |
| ATOM | 4747 | | LEU | 12 | 15.530 | 45.921 | 38.573 | 1.00 32.17 | CPS6 |
| ATOM | 4748 | C | LEU | 12 | 17.926 | 47.301 | 42.708 | 1.00 29.26 | CPS6 |
| ATOM | 4749 | 0 | LEU | 12 | 18.732 | 48.223 | 42.553 | 1.00 29.98 | CPS6 |
| ATOM | 4750 | N | ALA | 13 | 17.067 | 47.258 | 43.725 | 1.00 29.78 | CPS6 |
| ATOM | 4751 | CA | ALA | 13 | 17.027 | 48.315 | 44.733 | 1.00 30.29 | CPS6 |
| MOTA | 4752 | CB | ALA | 13 | 15.901 | 48.042 | 45.741 | 1.00 31.01 | CPS6 |
| ATOM | 4753 | C | ALA | 13 | 18.364 | 48.447 | 45.460 | 1.00 31.44 | CPS6 |
| MOTA | 4754 | 0 | ALA | 13 | 18.774 | 49.551 | 45.825 | 1.00 31.56 | CPS6 |
| MOTA | 4755 | N | ARG | 14 | 19.048 | 47.327 | 45.669 | 1.00 32.19 | CPS6 |
| MOTA | 4756 | CA | ARG | 14 | 20.338 | 47.357 | 46.352 | 1.00 32.76 | CPS6 |
| ATOM | 4757 | CB | ARG | 14 | 20.745 | 45.940 | 46.768 | 1.00 35.66 | CPS6 |
| ATOM | 4758 | CG | ARG | 14 | 22.097 | 45.852 | 47.437 | 1.00 39.95 | CPS6 |
| ATOM | 4759 | CD | ARG | 14 | 22.314 | 44.493 | 48.078 | 1.00 42.90 | CPS6 |
| ATOM | 4760 | NE | ARG | 14 | 23.727 | 44.261 | 48.363 | 1.00 46.95 | CPS6 |
| ATOM | 4761 | CZ | ARG | | 24.577 | 43.675 | 47.524 | 1.00 48.91 | CPS6 |
| | | | | 14 | | | | | |
| ATOM | 4762 | | ARG | 14 | 24.163 | 43.247 | 46.338 | 1.00 50.22 | CPS6 |
| ATOM | 4763 | | ARG | 14 | 25.850 | 43.523 | 47.868 | 1.00 50.46 | CPS6 |
| ATOM | 4764 | С | ARG | 14 | 21.415 | 48.002 | 45.469 | 1.00 32.36 | CPS6 |
| MOTA | 4765 | 0 | ARG | 14 | 22.268 | 48.747 | 45.961 | 1.00 31.82 | CPS6 |
| MOTA | 4766 | N | ILE | 15 | 21.381 | 47.719 | 44.171 | 1.00 31.44 | CPS6 |
| MOTA | 4767 | CA | ILE | 15 | 22.337 | 48.326 | 43.247 | 1.00 31.99 | CPS6 |
| MOTA | 4768 | CB | ILE | 15 | 22.153 | 47.777 | 41.817 | 1.00 32.07 | CPS6 |
| MOTA | 4769 | CG2 | ILE | 15 | 22.911 | 48.638 | 40.813 | 1.00 31.65 | CPS6 |
| ATOM | 4770 | CG1 | ILE | 15 | 22.655 | 46.333 | 41.752 | 1.00 32.16 | CPS6 |
| MOTA | 4771 | CD1 | ILE | 15 | 24.156 | 46.184 | 42.013 | 1.00 33.75 | CPS6 |
| ATOM | 4772 | С | ILE | 15 | 22.113 | 49.843 | 43.236 | 1.00 32.92 | CPS6 |
| ATOM | 4773 | ō | ILE | 15 | 23.062 | 50.627 | 43.265 | 1.00 32.09 | CPS6 |
| ATOM | 4774 | N | ALA | 16 | 20.851 | 50.254 | 43.201 | 1.00 33.77 | CPS6 |
| ATOM | 4775 | CA | ALA | 16 | 20.520 | 51.677 | 43.194 | 1.00 36.34 | CPS6 |
| | | | | | | 51.860 | 43.063 | 1.00 36.06 | CPS6 |
| ATOM | 4776 | CB | ALA | 16 | 19.014 | | | | CPS6 |
| ATOM | 4777 | C | ALA | 16 | 21.030 | 52.356 | 44.467 | 1.00 38.13 | |
| MOTA | 4778 | 0 | ALA | 16 | 21.491 | 53.498 | 44.427 | 1.00 38.48 | CPS6 |
| MOTA | 4779 | N | SER | 17 | 20.951 | 51.648 | 45.590 | 1.00 40.20 | CPS6 |
| MOTA | 4780 | CA | SER | 17 | 21.415 | 52.175 | 46.871 | 1.00 43.01 | CPS6 |
| MOTA | 4781 | CB | SER | 17 | 20.959 | 51.268 | 48.017 | 1.00 43.08 | CPS6 |
| ATOM | 4782 | OG | SER | 17 | 19.549 | 51.302 | 48.157 | 1.00 45.35 | CPS6 |
| ATOM | 4783 | C | SER | 17 | 22.934 | 52.320 | 46.919 | 1.00 44.34 | CPS6 |
| ATOM | 4784 | 0 | SER | 17 | 23.456 | 53.311 | 47.432 | 1.00 44.28 | CPS6 |
| MOTA | 4785 | N | MET | 18 | 23.644 | 51.323 | 46.402 | 1.00 45.43 | CPS6 |
| ATOM | 4786 | CA | MET | 18 | 25.100 | 51.370 | 46.390 | 1.00 47.02 | CPS6 |
| ATOM | 4787 | CB | MET | 18 | 25.678 | 50.035 | 45.917 | 1.00 48.11 | CPS6 |
| ALON | -1101 | CD | 1-175-7 | 10 | 23.070 | ددن. ت | ±3.3±1 | 2.00 20,22 | |

| ATOM | 4788 | CG | MET | 18 | 25.502 | 48.901 | 46.906 | 1.00 49.87 | CPS6 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| ATOM | 4789 | SD | MET | 18 | 26.307 | 47.401 | 46.338 | 1.00 54.02 | CPS6 |
| ATOM | 4790 | CE | MET | 18 | 24.997 | 46.663 | 45.390 | 1.00 52.20 | CPS6 |
| MOTA | 4791 | C | MET | 18 | 25.586 | 52.485 | 45.475 | 1.00 47.28 | CPS6 |
| MOTA | 4792 | 0 | MET | 18 | 26.533 | 53.196 | 45.799 | 1.00 47.27 | CPS6 |
| ATOM | 4793 | N | ALA | 19 | 24.923 | 52.636 | 44.334 | 1.00 47.27 | CPS6 |
| MOTA | 4794 | CA | ALA | 19 | 25.284 | 53.658 | 43.361 | 1.00 47.28 | |
| | | | | | | | | | CPS6 |
| ATOM | 4795 | CB | ALA | 19 | 24.558 | 53.397 | 42.049 | 1.00 47.94 | CPS6 |
| ATOM | 4796 | C | ALA | 19 | 24.956 | 55.059 | 43.867 | 1.00 49.67 | CPS6 |
| ATOM | 4797 | 0 | ALA | 19 | 25.644 | 56.031 | 43.539 | 1.00 48.84 | CPS6 |
| ATOM | 4798 | N | GLY | 20 | 23.895 | 55.159 | 44.659 | 1.00 50.28 | CPS6 |
| ATOM | 4799 | CA | GLY | 20 | 23.501 | 56.448 | 45.188 | 1.00 52.81 | CPS6 |
| ATOM | 4800 | С | GLY | 20 | 24.379 | 56.884 | 46.342 | 1.00 53.84 | CPS6 |
| MOTA | 4801 | 0 | GLY | 20 | 24.504 | 58.077 | 46.612 | 1.00 54.96 | CPS6 |
| ATOM | 4802 | N | ARG | 21 | 24.996 | 55.919 | 47.017 | 1.00 54.88 | CPS6 |
| ATOM | 4803 | CA | ARG | 21 | 25.853 | 56.215 | 48.157 | 1.00 56.13 | CPS6 |
| ATOM | 4804 | CB | ARG | 21 | 25.694 | 55.134 | 49.228 | 1.00 57.83 | CPS6 |
| ATOM | 4805 | CG | ARG | 21 | 24.308 | 55.086 | 49.857 | 1.00 60.18 | CPS6 |
| ATOM | 4806 | CD | ARG | 21 | 24.275 | 54.226 | 51.123 | 1.00 62.40 | CPS6 |
| MOTA | 4807 | NE | ARG | 21 | 24.085 | 52.797 | 50.866 | 1.00 64.82 | CPS6 |
| MOTA | 4808 | CZ | ARG | 21 | 25.003 | 51.979 | 50.352 | 1.00 65.81 | CPS6 |
| ATOM | 4809 | | ARG | 21 | 26.207 | 52.434 | 50.024 | 1.00 66.03 | CPS6 |
| ATOM | 4810 | NH2 | | 21 | 24.714 | 50.695 | 50.175 | 1.00 65.70 | CPS6 |
| ATOM | 4811 | C | ARG | 21 | 27.327 | 56.359 | 47.802 | 1.00 56.17 | CPS6 |
| ATOM | 4812 | 0 | ARG | 21 | 28.113 | 56.882 | 48.591 | 1.00 56.98 | CPS6 |
| ATOM | 4813 | N | GLN | 22 | 27.710 | 55.896 | 46.619 | 1.00 55.40 | CPS6 |
| ATOM | 4814 | CA | GLN | 22 | 29.104 | 55.992 | 46.207 | 1.00 54.24 | CPS6 |
| | | | | | | | 45.795 | 1.00 54.24 | CPS6 |
| ATOM | 4815 | CB | GLN | 22 | 29.637 | 54.619 | | 1.00 57.52 | CPS6 |
| ATOM | 4816 | CG | GLN | 22 | 29.456 | 53.533 | 46.836 | | |
| ATOM | 4817 | CD | GLN | 22 | 30.179 | 52.251 | 46.467 | 1.00 58.37 | CPS6 |
| ATOM | 4818 | | GLN | 22 | 30.060 | 51.236 | 47.154 | 1.00 59.62 | CPS6 |
| MOTA | 4819 | | GLN | 22 | 30.940 | 52.294 | 45.378 | 1.00 59.05 | CPS6 |
| MOTA | 4820 | С | GLN | 22 | 29.281 | 56.953 | 45.044 | 1.00 52.16 | CPS6 |
| MOTA | 4821 | 0 | GLN | 22 | 28.312 | 57.363 | 44.402 | 1.00 51.84 | CPS6 |
| MOTA | 4822 | N | LYS | 23 | 30.531 | 57.325 | 44.793 | 1.00 49.79 | CPS6 |
| ATOM | 4823 | CA | LYS | 23 | 30.848 | 58.203 | 43.679 | 1.00 47.03 | CPS6 |
| ATOM | 4824 | CB | LYS | 23 | 31.906 | 59.240 | 44.078 | 1.00 48.67 | CPS6 |
| ATOM | 4825 | CG | LYS | 23 | 32.117 | 60.319 | 43.025 | 1.00 50.00 | CPS6 |
| MOTA | 4826 | CD | LYS | 23 | 33.404 | 61.106 | 43.232 | 1.00 51.39 | CPS6 |
| ATOM | 4827 | CE | LYS | 23 | 33.384 | 61.925 | 44.506 | 1.00 52.42 | CPS6 |
| ATOM | 4828 | NZ | LYS | 23 | 34.570 | 62.835 | 44.558 | 1.00 53.74 | CPS6 |
| ATOM | 4829 | C | LYS | 23 | 31.406 | 57.280 | 42.595 | 1.00 43.64 | CPS6 |
| ATOM | 4830 | 0 | LYS | 23 | 32.259 | 56.433 | 42.866 | 1.00 43.39 | CPS6 |
| ATOM | 4831 | N | ARG | 24 | 30.898 | 57.421 | 41.379 | 1.00 40.62 | CPS6 |
| ATOM | 4832 | CA | ARG | 24 | 31.363 | 56.603 | 40.266 | 1.00 38.09 | CPS6 |
| MOTA | 4833 | СВ | ARG | 24 | 32.806 | 56.991 | 39.919 | 1.00 38.24 | CPS6 |
| ATOM | 4834 | CG | ARG | 24 | 32.935 | 58.400 | 39.340 | 1.00 38.55 | CPS6 |
| ATOM | 4835 | CD | ARG | 24 | 34.348 | 58.672 | 38.853 | 1.00 38.30 | CPS6 |
| MOTA | 4836 | NE | ARG | 24 | 35.297 | 58.859 | 39.948 | 1.00 39.05 | CPS6 |
| ATOM | 4837 | CZ | ARG | 24 | 35.511 | 60.019 | 40.561 | 1.00 39.71 | CPS6 |
| | | | | | 34.846 | 61.108 | 40.190 | 1.00 39.71 | CPS6 |
| ATOM | 4838 | | ARG | 24 | | | 40.190 | 1.00 39.47 | CPS6 |
| ATOM | 4839 | | ARG | 24 | 36.396 | 60.092 | | | CPS6 |
| ATOM | 4840 | С | ARG | 24 | 31.266 | 55.086 | 40.500 | 1.00 35.99 | |
| ATOM | 4841 | 0 | ARG | 24 | 32.202 | 54.339 | 40.206 | 1.00 34.55 | CPS6 |
| ATOM | 4842 | N | PHE | 25 | 30.135 | 54.627 | 41.026 | 1.00 33.55 | CPS6 |
| ATOM | 4843 | CA | PHE | 25 | 29.959 | 53.196 | 41.251 | 1.00 31.77 | CPS6 |
| ATOM | 4844 | CB | PHE | 25 | 28.647 | 52.938 | 42.012 | 1.00 32.24 | CPS6 |

| ATOM | 4845 | CG | PHE | 25 | 28.331 | 51.481 | 42.211 | 1.00 31.39 | CPS6 |
|------|------|-----|-----|----|--------|--------|--------|------------|-------|
| | | | | | 27.306 | | | | |
| ATOM | 4846 | CD1 | | 25 | | 50.879 | 41.495 | 1.00 33.76 | CP\$6 |
| MOTA | 4847 | CD2 | | 25 | 29.069 | 50.709 | 43.102 | 1.00 32.67 | CPS6 |
| MOTA | 4848 | CE1 | | 25 | 27.021 | 49.524 | 41.663 | 1.00 32.84 | CPS6 |
| ATOM | 4849 | CE2 | PHE | 25 | 28.794 | 49.354 | 43.277 | 1.00 32.53 | CPS6 |
| ATOM | 4850 | CZ | PHE | 25 | 27.764 | 48.763 | 42.553 | 1.00 32.75 | CPS6 |
| ATOM | 4851 | C | PHE | 25 | 29.943 | 52.489 | 39.887 | 1.00 30.17 | CPS6 |
| ATOM | 4852 | 0 | PHE | 25 | 30.573 | 51.446 | 39.706 | 1.00 28.44 | CPS6 |
| ATOM | 4853 | | ALA | 26 | 29.236 | 53.074 | 38.923 | 1.00 29.20 | CPS6 |
| | | N | | | | | | | |
| MOTA | 4854 | CA | ALA | 26 | 29.158 | 52.484 | 37.592 | 1.00 28.94 | CPS6 |
| MOTA | 4855 | CB | ALA | 26 | 28.244 | 53.319 | 36.697 | 1.00 29.36 | CPS6 |
| ATOM | 4856 | C | ALA | 26 | 30.540 | 52.376 | 36.961 | 1.00 28.91 | CPS6 |
| ATOM | 4857 | 0 | ALA | 26 | 30.857 | 51.378 | 36.325 | 1.00 26.93 | CPS6 |
| ATOM | 4858 | N | GLU | 27 | 31.358 | 53.411 | 37.144 | 1.00 28.69 | CPS6 |
| ATOM | 4859 | CA | GLU | 27 | 32.701 | 53.434 | 36.576 | 1.00 29.76 | CPS6 |
| ATOM | 4860 | CB | GLU | 27 | 33.317 | 54.829 | 36.730 | 1.00 30.26 | CPS6 |
| MOTA | 4861 | CG | GLU | 27 | 32.737 | 55.916 | 35.822 | 1.00 32.04 | CPS6 |
| ATOM | 4862 | CD | GLU | 27 | 31.325 | 56.344 | 36.195 | 1.00 33.96 | CPS6 |
| | | | GLU | | 30.902 | | 37.353 | | CPS6 |
| ATOM | 4863 | | | 27 | | 56.135 | | 1.00 32.41 | |
| ATOM | 4864 | OE2 | | 27 | 30.638 | 56.914 | 35.318 | 1.00 37.48 | CPS6 |
| ATOM | 4865 | С | GLU | 27 | 33.622 | 52.399 | 37.224 | 1.00 29.59 | CPS6 |
| MOTA | 4866 | 0 | GLU | 27 | 34.661 | 52.040 | 36.673 | 1.00 29.53 | CPS6 |
| MOTA | 4867 | N | ARG | 28 | 33.243 | 51.927 | 38.402 | 1.00 30.48 | CPS6 |
| MOTA | 4868 | CA | ARG | 28 | 34.040 | 50.934 | 39.107 | 1.00 32.10 | CPS6 |
| ATOM | 4869 | CB | ARG | 28 | 33.782 | 51.051 | 40.611 | 1.00 35.59 | CPS6 |
| ATOM | 4870 | CG | ARG | 28 | 34.480 | 50.013 | 41.467 | 1.00 40.15 | CPS6 |
| ATOM | 4871 | CD | ARG | 28 | 34.042 | 50.172 | 42.911 | 1.00 44.70 | CPS6 |
| ATOM | 4872 | NE | ARG | 28 | 33.719 | 48.891 | 43.529 | 1.00 48.06 | CPS6 |
| | | CZ | ARG | 28 | 33.004 | 48.764 | 44.642 | 1.00 50.43 | CPS6 |
| MOTA | 4873 | | | | | | | 1.00 50.45 | CPS6 |
| MOTA | 4874 | | ARG | 28 | 32.535 | 49.845 | 45.258 | | CPS6 |
| ATOM | 4875 | | ARG | 28 | 32.755 | 47.558 | 45.139 | 1.00 51.52 | |
| MOTA | 4876 | C | ARG | 28 | 33.677 | 49.526 | 38.621 | 1.00 30.71 | CPS6 |
| ATOM | 4877 | 0 | ARG | 28 | 34.546 | 48.659 | 38.464 | 1.00 32.13 | CPS6 |
| ATOM | 4878 | N | ILE | 29 | 32.391 | 49.316 | 38.364 | 1.00 28.03 | CPS6 |
| MOTA | 4879 | CA | ILE | 29 | 31.891 | 48.016 | 37.922 | 1.00 26.37 | CPS6 |
| MOTA | 4880 | CB | ILE | 29 | 30.387 | 47.854 | 38.270 | 1.00 25.85 | CPS6 |
| ATOM | 4881 | CG2 | ILE | 29 | 29.886 | 46.496 | 37.802 | 1.00 25.90 | CPS6 |
| ATOM | 4882 | CG1 | | 29 | 30.164 | 48.051 | 39.776 | 1.00 27.54 | CPS6 |
| ATOM | 4883 | CD1 | | 29 | 30.962 | 47.113 | 40.667 | 1.00 27.66 | CPS6 |
| | | | | 29 | | 47.746 | 36.421 | 1.00 25.65 | CPS6 |
| ATOM | 4884 | C | ILE | | 32.030 | | | 1.00 24.93 | CPS6 |
| MOTA | 4885 | 0 | ILE | 29 | 32.327 | 46.617 | 36.017 | | CPS6 |
| MOTA | 4886 | N | LEU | 30 | 31.820 | 48.784 | 35.609 | 1.00 23.77 | |
| MOTA | 4887 | CA | LEU | 30 | 31.844 | 48.651 | 34.158 | 1.00 24.32 | CPS6 |
| MOTA | 4888 | CB | LEU | 30 | 30.665 | 49.429 | 33.567 | 1.00 24.16 | CPS6 |
| MOTA | 4889 | CG | LEU | 30 | 29.282 | 49.141 | 34.169 | 1.00 25.20 | CPS6 |
| MOTA | 4890 | CD1 | LEU | 30 | 28.251 | 50.068 | 33.540 | 1.00 24.33 | CPS6 |
| MOTA | 4891 | CD2 | LEU | 30 | 28.898 | 47.695 | 33.927 | 1.00 23.57 | CPS6 |
| MOTA | 4892 | С | LEU | 30 | 33.121 | 49.071 | 33.433 | 1.00 24.24 | CPS6 |
| ATOM | 4893 | ō | LEU | 30 | 33.820 | 49.996 | 33.845 | 1.00 23.43 | CPS6 |
| | 4894 | | | 31 | 33.404 | 48.376 | 32.341 | 1.00 23.91 | CPS6 |
| ATOM | | N | THR | | | | | 1.00 25.21 | CPS6 |
| ATOM | 4895 | CA | THR | 31 | 34.573 | 48.676 | 31.523 | | CPS6 |
| MOTA | 4896 | CB | THR | 31 | 34.999 | 47.461 | 30.695 | 1.00 25.51 | |
| MOTA | 4897 | | THR | 31 | 33.972 | 47.150 | 29.739 | 1.00 24.34 | CPS6 |
| MOTA | 4898 | CG2 | THR | 31 | 35.245 | 46.265 | 31.597 | | CPS6 |
| ATOM | 4899 | С | THR | 31 | 34.219 | 49.798 | 30.553 | | CPS6 |
| ATOM | 4900 | 0 | THR | 31 | 33.071 | 50.247 | 30.490 | 1.00 25.37 | CPS6 |
| ATOM | 4901 | N | ARG | 32 | 35.202 | 50.240 | 29.782 | | CPS6 |
| ALON | | •• | | | | | | | |

| 3.0004 | 4000 | ~ 3 | 350 | 2.2 | 34 076 | 5- 310 | 22 212 | | |
|--------|------|------------|-----|-----|--------|--------|--------|------------|------|
| MOTA | 4902 | CA | ARG | 32 | 34.976 | 51.310 | 28.818 | 1.00 29.54 | CPS6 |
| ATOM | 4903 | CB | ARG | 32 | 36.290 | 51.626 | 28.091 | 1.00 32.98 | CPS6 |
| ATOM | 4904 | CG | ARG | 32 | 36.198 | 52.721 | 27.040 | 1.00 38.34 | CPS6 |
| ATOM | 4905 | CD | ARG | 32 | 37.595 | 53.116 | 26.557 | 1.00 42.64 | CPS6 |
| ATOM | 4906 | NE | ARG | 32 | 38.282 | 53.987 | 27.513 | 1.00 45.62 | CPS6 |
| ATOM | 4907 | CZ | ARG | 32 | 38,009 | 55.281 | 27.677 | 1.00 47.09 | CPS6 |
| ATOM | 4908 | NH1 | | 32 | 37.065 | 55.865 | 26.946 | 1.00 48.54 | CPS6 |
| ATOM | 4909 | NH2 | | 32 | | | | | |
| | | | | | 38.675 | 55.992 | 28.576 | 1.00 48.16 | CPS6 |
| ATOM | 4910 | C | ARG | 32 | 33.879 | 50.928 | 27.815 | 1.00 28.32 | CPS6 |
| MOTA | 4911 | 0 | ARG | 32 | 32.969 | 51.711 | 27.544 | 1.00 27.76 | CPS6 |
| MOTA | 4912 | N | SER | 33 | 33.966 | 49.719 | 27.275 | 1.00 27.75 | CPS6 |
| ATOM | 4913 | CA | SER | 33 | 32.988 | 49.238 | 26.303 | 1.00 28.81 | CPS6 |
| ATOM | 4914 | CB | SER | 33 | 33.386 | 47.828 | 25.835 | 1.00 30.61 | CPS6 |
| ATOM | 4915 | 0G | SER | 33 | 32.421 | 47.266 | 24.963 | 1.00 33.62 | CPS6 |
| ATOM | 4916 | C | SER | 33 | 31.586 | 49.211 | 26.926 | 1.00 28.93 | CPS6 |
| ATOM | 4917 | ō | SER | 33 | 30.599 | 49.614 | 26.302 | 1.00 28.74 | CPS6 |
| ATOM | 4918 | N | GLU | 34 | 31.508 | 48.733 | 28.160 | 1.00 26.50 | CPS6 |
| | | | | | | | | | |
| ATOM | 4919 | CA | GLU | 34 | 30.237 | 48.650 | 28.866 | 1.00 27.17 | CPS6 |
| MOTA | 4920 | CB | GLU | 34 | 30.405 | 47.814 | 30.137 | 1.00 25.92 | CPS6 |
| MOTA | 4921 | CG | GLU | 34 | 30.649 | 46.339 | 29.830 | 1.00 25.85 | CPS6 |
| MOTA | 4922 | CD | GLU | 34 | 30.989 | 45.521 | 31.064 | 1.00 25.48 | CPS6 |
| ATOM | 4923 | OE1 | GLU | 34 | 30.771 | 44.290 | 31.035 | 1.00 24.91 | CPS6 |
| ATOM | 4924 | OE2 | GLU | 34 | 31.479 | 46.102 | 32.057 | 1.00 23.64 | CPS6 |
| ATOM | 4925 | С | GLU | 34 | 29.688 | 50.029 | 29.193 | 1.00 27.92 | CPS6 |
| ATOM | 4926 | 0 | GLU | 34 | 28.492 | 50.276 | 29.026 | 1.00 28.34 | CPS6 |
| ATOM | 4927 | N | LEU | 35 | 30.556 | 50.929 | 29.648 | 1.00 27.84 | CPS6 |
| ATOM | 4928 | CA | LEU | 35 | 30.137 | 52.286 | 29.977 | 1.00 30.69 | CPS6 |
| ATOM | 4929 | CB | LEU | 35 | 31.310 | 53.081 | 30.557 | 1.00 30.33 | CPS6 |
| | | | | | | | | 1.00 30.63 | CPS6 |
| ATOM | 4930 | CG | LEU | 35 | 31.719 | 52.712 | 31.981 | | |
| MOTA | 4931 | | LEU | 35 | 33.062 | 53.354 | 32.327 | 1.00 30.22 | CPS6 |
| MOTA | 4932 | | LEU | 35 | 30.631 | 53.170 | 32.943 | 1.00 30.10 | CPS6 |
| MOTA | 4933 | С | LEU | 35 | 29.583 | 53.012 | 28.756 | 1.00 32.12 | CPS6 |
| MOTA | 4934 | 0 | LEU | 35 | 28.669 | 53.826 | 28.880 | 1.00 32.67 | CPS6 |
| MOTA | 4935 | N | ASP | 36 | 30.140 | 52.730 | 27.579 | 1.00 34.02 | CPS6 |
| MOTA | 4936 | CA | ASP | 36 | 29.656 | 53.376 | 26.362 | 1.00 36.28 | CPS6 |
| ATOM | 4937 | CB | ASP | 36 | 30.457 | 52.928 | 25.131 | 1.00 38.02 | CPS6 |
| ATOM | 4938 | CG | ASP | 36 | 31.801 | 53.636 | 25.016 | 1.00 41.17 | CPS6 |
| ATOM | 4939 | | ASP | 36 | 31.924 | 54.767 | 25.538 | 1.00 42.30 | CPS6 |
| ATOM | 4940 | | ASP | 36 | 32.730 | 53.073 | 24.391 | 1.00 43.23 | CPS6 |
| ATOM | 4941 | C | ASP | 36 | 28.177 | 53.071 | 26.152 | 1.00 37.04 | CPS6 |
| ATOM | 4942 | 0 | ASP | 36 | 27.411 | 53.945 | 25.756 | 1.00 38.21 | CPS6 |
| | | | | | | | | 1.00 36.14 | CPS6 |
| ATOM | 4943 | N | GLN | 37 | 27.772 | 51.836 | 26.427 | | CPS6 |
| MOTA | 4944 | CA | GLN | 37 | 26.376 | 51.449 | 26.261 | 1.00 37.10 | |
| MOTA | 4945 | CB | GLN | 37 | 26.253 | 49.928 | 26.271 | 1.00 39.04 | CPS6 |
| MOTA | 4946 | CG | GLN | 37 | 27.296 | 49.234 | 25.424 | 1.00 43.60 | CPS6 |
| MOTA | 4947 | CD | GLN | 37 | 27.084 | 47.741 | 25.357 | 1.00 47.47 | CPS6 |
| MOTA | 4948 | 0E1 | GLN | 37 | 26.134 | 47.268 | 24.726 | 1.00 50.58 | CPS6 |
| ATOM | 4949 | NE2 | GLN | 37 | 27.960 | 46.983 | 26.016 | 1.00 47.62 | CPS6 |
| ATOM | 4950 | C | GLN | 37 | 25.535 | 52.042 | 27.389 | 1.00 36.39 | CPS6 |
| ATOM | 4951 | ō | GLN | 37 | 24.466 | 52.607 | 27.159 | 1.00 36.41 | CPS6 |
| | | | | 38 | 26.045 | 51.909 | 28.608 | 1.00 35.09 | CPS6 |
| MOTA | 4952 | N | TYR | | | | | 1.00 35.03 | CPS6 |
| ATOM | 4953 | CA | TYR | 38 | 25.395 | 52.405 | 29.813 | | CPS6 |
| ATOM | 4954 | CB | TYR | 38 | 26.346 | 52.199 | 31.000 | 1.00 33.56 | |
| MOTA | 4955 | CG | TYR | 38 | 25.868 | 52.724 | 32.330 | 1.00 32.55 | CPS6 |
| MOTA | 4956 | CD1 | TYR | 38 | 26.296 | 53.958 | 32.810 | 1.00 32.33 | CPS6 |
| MOTA | 4957 | CE1 | TYR | 38 | 25.882 | 54.427 | 34.057 | 1.00 33.78 | CPS6 |
| ATOM | 4958 | CD2 | TYR | 38 | 25.008 | 51.969 | 33.127 | 1.00 31.82 | CPS6 |
| | | | | | | | | | |

| 35034 | 4050 | ana | mr.r | 3.0 | 24 500 | | 2 . 2 | | |
|-------|------|-----|----------------|-----|--------|--------|--------|------------|-------|
| ATOM | 4959 | CE2 | TYR | 38 | 24.590 | 52.423 | 34.367 | 1.00 32.17 | CPS6 |
| ATOM | 4960 | CZ | TYR | 38 | 25.029 | 53.652 | 34.829 | 1.00 33.51 | CPS6 |
| ATOM | 4961 | OH | TYR | 38 | 24.611 | 54.099 | 36.060 | 1.00 34.37 | CPS6 |
| ATOM | 4962 | C | TYR | 38 | 24.978 | 53.872 | 29.714 | 1.00 36.19 | CPS6 |
| ATOM | 4963 | 0 | TYR | 38 | 23.825 | 54.213 | 29.974 | 1.00 35.32 | CPS6 |
| MOTA | 4964 | N | TYR | 39 | 25.917 | 54.733 | 29.335 | 1.00 37.73 | CPS6 |
| ATOM | 4965 | CA | TYR | 39 | 25.649 | 56.168 | 29.229 | 1.00 39.75 | CPS6 |
| | | | | | | | | | |
| ATOM | 4966 | CB | TYR | 39 | 26.922 | 56.925 | 28.838 | 1.00 39.88 | CPS6 |
| MOTA | 4967 | CG | TYR | 39 | 28.029 | 56.896 | 29.873 | 1.00 40.44 | CPS6 |
| MOTA | 4968 | CD1 | TYR | 39 | 27.742 | 56.963 | 31.239 | 1.00 39.77 | CPS6 |
| ATOM | 4969 | CE1 | TYR | 39 | 28.762 | 56.991 | 32.188 | 1.00 39.44 | CPS6 |
| ATOM | 4970 | CD2 | TYR | 39 | 29.370 | 56.855 | 29.481 | 1.00 40.21 | CPS6 |
| ATOM | 4971 | CE2 | TYR | 39 | 30.399 | 56.884 | 30.420 | 1.00 39.93 | CPS6 |
| ATOM | 4972 | CZ | TYR | 39 | 30.089 | 56.954 | 31.773 | 1.00 40.43 | CPS6 |
| ATOM | 4973 | OH | TYR | 39 | 31.109 | 57.010 | 32.702 | 1.00 40.54 | |
| | | | | | | | | | CPS6 |
| ATOM | 4974 | C | TYR | 39 | 24.538 | 56.546 | 28.254 | 1.00 41.06 | CPS6 |
| MOTA | 4975 | 0 | TYR | 39 | 23.957 | 57.627 | 28.357 | 1.00 42.29 | CPS6 |
| ATOM | 4976 | N | GLU | 40 | 24.239 | 55.668 | 27.307 | 1.00 42.33 | CPS6 |
| MOTA | 4977 | CA | GLU | 40 | 23.199 | 55.965 | 26.331 | 1.00 44.33 | CPS6 |
| MOTA | 4978 | CB | GLU | 40 | 23.541 | 55.323 | 24.986 | 1.00 46.05 | CPS6 |
| ATOM | 4979 | CG | GLU | 40 | 24.916 | 55.689 | 24.466 | 1.00 50.15 | CPS6 |
| ATOM | 4980 | CD | GLU | 40 | 25.203 | 55.088 | 23.105 | 1.00 52.92 | CPS6 |
| ATOM | 4981 | | GLU | 40 | 25.040 | 53.857 | 22.948 | 1.00 55.32 | CPS6 |
| ATOM | 4982 | | GLU | 40 | 25.599 | 55.848 | 22.191 | 1.00 54.91 | CPS6 |
| ATOM | 4983 | C | GLU | | 21.827 | 55.488 | 26.780 | 1.00 34.31 | CPS6 |
| | | | | 40 | | | | | |
| ATOM | 4984 | 0 | GLU | 40 | 20.854 | 55.629 | 26.041 | 1.00 44.77 | CPS6 |
| ATOM | 4985 | N | LEU | 41 | 21.743 | 54.941 | 27.991 | 1.00 42.63 | CPS6 |
| ATOM | 4986 | CA | LEU | 41 | 20.474 | 54.427 | 28.499 | 1.00 42.23 | CPS6 |
| MOTA | 4987 | CB | LEU | 41 | 20.696 | 53.114 | 29.259 | 1.00 41.12 | CPS6 |
| MOTA | 4988 | CG | LEU | 41 | 21.294 | 51.934 | 28.486 | 1.00 40.93 | CP\$6 |
| ATOM | 4989 | CD1 | LEU | 41 | 21.524 | 50.777 | 29.446 | 1.00 39.97 | CPS6 |
| MOTA | 4990 | CD2 | LEU | 41 | 20.362 | 51.514 | 27.360 | 1.00 40.04 | CPS6 |
| MOTA | 4991 | C | LEU | 41 | 19.736 | 55.392 | 29.410 | 1.00 41.84 | CPS6 |
| ATOM | 4992 | 0 | LEU | 41 | 20.317 | 56.335 | 29.934 | 1.00 41.86 | CPS6 |
| ATOM | 4993 | N | SER | 42 | 18.447 | 55.129 | 29.597 | 1.00 42.32 | CPS6 |
| ATOM | 4994 | CA | SER | 42 | 17.602 | 55.937 | 30.465 | 1.00 43.65 | CPS6 |
| | | | | | | | 30.252 | 1.00 43.85 | CPS6 |
| ATOM | 4995 | CB | SER | 42 | 16.134 | 55.578 | | | |
| ATOM | 4996 | OG | SER | 42 | 15.871 | 54.269 | 30.726 | 1.00 44.29 | CPS6 |
| MOTA | 4997 | C | SER | 42 | 17.983 | 55.620 | 31.902 | 1.00 43.88 | CPS6 |
| MOTA | 4998 | 0 | SER | 42 | 18.661 | 54.626 | 32.157 | 1.00 44.22 | CPS6 |
| ATOM | 4999 | N | \mathtt{GLU} | 43 | 17.540 | 56.447 | 32.843 | 1.00 43.94 | CPS6 |
| MOTA | 5000 | CA | GLU | 43 | 17.860 | 56.216 | 34.248 | 1.00 44.69 | CPS6 |
| MOTA | 5001 | CB | GLU | 43 | 17.195 | 57.266 | 35.147 | 1.00 47.52 | CPS6 |
| MOTA | 5002 | CG | GLU | 43 | 17.466 | 57.033 | 36.632 | 1.00 51.04 | CPS6 |
| ATOM | 5003 | CD | GLU | 43 | 16.733 | 58.002 | 37.546 | 1.00 53.92 | CPS6 |
| ATOM | 5004 | | GLU | 43 | 15.480 | 57.965 | 37.596 | 1.00 55.09 | CPS6 |
| | | | | | | | | 1.00 55.13 | CPS6 |
| ATOM | 5005 | | GLU | 43 | 17.418 | 58.802 | 38.221 | | |
| ATOM | 5006 | C | GLU | 43 | 17.411 | 54.828 | 34.687 | 1.00 43.76 | CPS6 |
| ATOM | 5007 | 0 | GLU | 43 | 18.123 | 54.143 | 35.419 | 1.00 43.62 | CPS6 |
| ATOM | 5008 | N | LYS | 44 | 16.227 | 54.419 | 34.244 | 1.00 42.65 | CPS6 |
| MOTA | 5009 | CA | LYS | 44 | 15.699 | 53.110 | 34.601 | 1.00 42.18 | CPS6 |
| MOTA | 5010 | CB | LYS | 44 | 14.244 | 52.980 | 34.151 | 1.00 43.86 | CPS6 |
| MOTA | 5011 | CG | LYS | 44 | 13.612 | 51.643 | 34.508 | 1.00 45.75 | CPS6 |
| MOTA | 5012 | CD | LYS | 44 | 12.155 | 51.590 | 34.086 | 1.00 47.40 | CPS6 |
| ATOM | 5013 | CE | LYS | 44 | 11.521 | 50.267 | 34.474 | 1.00 48.83 | CPS6 |
| ATOM | 5013 | NZ | LYS | 44 | 10.076 | 50.213 | 34.107 | 1.00 50.91 | CPS6 |
| | | | | | | | 33.966 | 1.00 40.95 | CPS6 |
| MOTA | 5015 | C | LYS | 44 | 16.521 | 51.994 | 33.700 | 1.00 40.99 | C2-00 |

| MOTA | 5016 | 0 | LYS | 44 | 16.952 | 51.064 | 34.645 | 1.00 40.09 | CPS6 |
|------|-----------------------|--------|------------|----------|--------|--------|--------|--------------------------|------|
| MOTA | 5017 | N | ARG | 45 | 16.722 | 52.091 | 32.656 | 1.00 39.93 | CPS6 |
| ATOM | 5018 | CA | ARG | 45 | 17.490 | 51.095 | 31.923 | 1.00 38.26 | CPS6 |
| MOTA | 5019 | CB | ARG | 45 | 17.518 | 51.437 | 30.434 | 1.00 40.94 | CPS6 |
| MOTA | 5020 | CG | ARG | 45 | 16.178 | 51.285 | 29.736 | 1.00 45.37 | CPS6 |
| ATOM | 5021 | CD | ARG | 45 | 15.796 | 49.825 | 29.572 | 1.00 48.47 | CPS6 |
| ATOM | 5022 | NE | ARG | 45 | 16.746 | 49.092 | 28.732 | 1.00 52.03 | CPS6 |
| MOTA | 5023 | CZ | ARG | 45 | 17.047 | 49.411 | 27.475 | 1.00 54.07 | CPS6 |
| ATOM | 5024 | NH1 | ARG | 45 | 16.480 | 50.459 | 26.888 | 1.00 55.15 | CPS6 |
| MOTA | 5025 | NH2 | ARG | 45 | 17.917 | 48.672 | 26.796 | 1.00 55.63 | CPS6 |
| MOTA | 5026 | С | ARG | 45 | 18.915 | 50.992 | 32.441 | 1.00 35.74 | CPS6 |
| MOTA | 5027 | 0 | ARG | 45 | 19.524 | 49.926 | 32.374 | 1.00 33.44 | CPS6 |
| ATOM | 5028 | N | LYS | 46 | 19.456 | 52.098 | 32.945 | 1.00 33.77 | CPS6 |
| ATOM | 5029 | CA | LYS | 46 | 20.814 | 52.075 | 33.466 | 1.00 32.86 | CPS6 |
| ATOM | 5030 | CB | LYS | 46 | 21.311 | 53.489 | 33.787 | 1.00 33.65 | CPS6 |
| ATOM | 5031 | CG | LYS | 46 | 21.636 | 54.270 | 32.529 | 1.00 35.15 | CPS6 |
| ATOM | 5032 | CD | LYS | 46 | 22.700 | 55.318 | 32.752 | 1.00 38.55 | CPS6 |
| MOTA | 5033 | CE | LYS | 46 | 22.185 | 56.492 | 33.528 | 1.00 38.97 | CPS6 |
| ATOM | 5034 | NZ | LYS | 46 | 22.923 | 57.716 | 33.075 | 1.00 40.88 | CPS6 |
| ATOM | 5035 | C | LYS | 46 | 20.904 | 51.196 | 34.693 | 1.00 31.44 | CPS6 |
| ATOM | 5036 | ō | LYS | 46 | 21.841 | 50.415 | 34.832 | 1.00 30.69 | CPS6 |
| ATOM | 5037 | N | ASN | 47 | 19.927 | 51.310 | 35.585 | 1.00 30.34 | CPS6 |
| ATOM | 5038 | CA | ASN | 47 | 19.935 | 50.486 | 36.788 | 1.00 29.82 | CPS6 |
| ATOM | 5039 | CB | ASN | 47 | 18.779 | 50.880 | 37.713 | 1.00 30.59 | CPS6 |
| ATOM | 5040 | CG | ASN | 47 | 18.683 | 49.983 | 38.935 | 1.00 32.30 | CPS6 |
| ATOM | 5041 | | ASN | 47 | 19.510 | 50.057 | 39.851 | 1.00 32.30 | CPS6 |
| ATOM | 5042 | | ASN | 47 | 17.675 | 49.119 | 38.950 | 1.00 34.07 | CPS6 |
| ATOM | 5042 | C | ASN | 47 | 19.821 | 49.003 | 36.401 | 1.00 28.64 | CPS6 |
| ATOM | 5044 | 0 | ASN | 47 | 20.503 | 48.154 | 36.970 | 1.00 28.65 | CPS6 |
| ATOM | 5045 | N | GLU | 48 | 18.972 | 48.700 | 35.424 | 1.00 28.08 | CPS6 |
| ATOM | 5045 | CA | GLU | 48 | 18.796 | 47.319 | 34.969 | 1.00 28.15 | CPS6 |
| ATOM | 5047 | CB | GLU | 48 | 17.680 | 47.234 | 33.927 | 1.00 31.68 | CPS6 |
| ATOM | 5048 | CG | GLU | 48 | 16.301 | 47.618 | 34.448 | 1.00 36.94 | CPS6 |
| MOTA | 5049 | CD | GLU | 48 | 15.246 | 47.631 | 33.352 | 1.00 40.49 | CPS6 |
| ATOM | 5050 | | GLU | 48 | 14.076 | 47.950 | 33.661 | 1.00 42.57 | CPS6 |
| MOTA | 5051 | | GLU | 48 | 15.585 | 47.325 | 32.185 | 1.00 40.94 | CPS6 |
| MOTA | 5052 | C | GLU | 48 | 20.085 | 46.783 | 34.344 | 1.00 27.02 | CPS6 |
| ATOM | 5053 | 0 | GLU | 48 | 20.489 | 45.646 | 34.598 | 1.00 25.06 | CPS6 |
| ATOM | 5054 | N | PHE | 49 | 20.714 | 47.613 | 33.515 | 1.00 25.48 | CPS6 |
| ATOM | 5055 | CA | PHE | 49 | 21.949 | 47.243 | 32.830 | 1.00 26.00 | CPS6 |
| ATOM | 5056 | CB | PHE | 49 | 22.351 | 48.358 | 31.858 | 1.00 26.69 | CPS6 |
| MOTA | 5057 | CG | PHE | 49 | 23.585 | 48.058 | 31.057 | 1.00 27.23 | CPS6 |
| MOTA | 5058 | | PHE | 49 | 23.497 | 47.397 | 29.838 | 1.00 28.29 | CPS6 |
| ATOM | 5059 | | PHE | 49 | 24.835 | 48.455 | 31.515 | 1.00 26.82 | CPS6 |
| ATOM | 5060 | | PHE | 49 | 24.633 | 47.142 | 29.081 | 1.00 28.93 | CPS6 |
| ATOM | 5061 | | PHE | 49 | 25.987 | 48.202 | 30.765 | 1.00 27.94 | CPS6 |
| | | CZ | PHE | 49 | 25.886 | 47.548 | 29.550 | 1.00 28.38 | CPS6 |
| ATOM | 5062 | C | | 49 | 23.066 | 46.997 | 33.837 | 1.00 24.84 | CPS6 |
| ATOM | 5063 | | PHE | | 23.739 | 45.966 | 33.789 | 1.00 25.50 | CPS6 |
| MOTA | 5064 50 6 5 | N O | PHE LEU | 49 50 | 23.739 | 47.946 | 34.747 | 1.00 23.30 | CPS6 |
| ATOM | | | | | 24.296 | 47.824 | 35.773 | 1.00 24.10 | CPS6 |
| ATOM | 5066 | CA | LEU | 50 50 | | | | 1.00 22.37 | CPS6 |
| ATOM | 5067 | CB | LEU | 50 | 24.304 | 49.088 | 36.647 | 1.00 24.37 | CPS6 |
| ATOM | 5068 | CG | LEU | 50 | 25.348 | 49.178 | 37.759 | | CPS6 |
| MOTA | 5069 | | LEU | 50 | 26.760 | 49.145 | 37.149 | 1.00 26.03 1.00 26.29 | CPS6 |
| MOTA | 5070 | | LEU | 50 | 25.141 | 50.471 | 38.537 | | CPS6 |
| MOTA | 5071 | C | LEU | 50 | 24.081 | 46.583 | 36.653 | 1.00 21.87 1.00 21.43 | CPS6 |
| ATOM | 5072 | 0 | LEU | 50 | 25.022 | 45.839 | 36.939 | 1.00 21.43 | CFOO |
| | | | | | | | | | |

| ATOM | 5073 | N | ALA | 51 | 22.844 | 46.364 | 37.089 | 1.00 21.05 | CPS6 |
|------|------|-----|-----|------------|--------|--------|--------|------------|------|
| ATOM | 5074 | CA | ALA | 51 | 22.524 | 45.218 | 37.940 | 1.00 21.01 | CPS6 |
| ATOM | 5075 | CB | ALA | 51 | 21.038 | 45.271 | 38.346 | 1.00 20.12 | CPS6 |
| ATOM | 5076 | C | ALA | 51 | 22.829 | 43.894 | 37.223 | 1.00 20.25 | CPS6 |
| ATOM | 5077 | 0 | ALA | 51 | 23.351 | 42.955 | 37.825 | 1.00 20.85 | CPS6 |
| MOTA | 5078 | N | GLY | 52 | 22.493 | 43.830 | 35,943 | 1.00 21.02 | CPS6 |
| ATOM | 5079 | CA | GLY | 52 | 22.742 | 42.624 | 35.164 | 1.00 20.99 | CPS6 |
| ATOM | | C | GLY | 52 | 24.232 | 42.376 | 34.989 | 1.00 22.24 | CPS6 |
| | 5080 | | | | | | | | |
| ATOM | 5081 | 0 | GLY | 52 | 24.688 | 41.232 | 35.044 | 1.00 21.77 | CPS6 |
| MOTA | 5082 | И | ARG | 53 | 24.992 | 43.444 | 34.764 | 1.00 22.45 | CPS6 |
| MOTA | 5083 | CA | ARG | 53 | 26.442 | 43.317 | 34.600 | 1.00 22.02 | CPS6 |
| MOTA | 5084 | CB | ARG | 53 | 27.051 | 44.624 | 34.093 | 1.00 23.58 | CPS6 |
| MOTA | 5085 | CG | ARG | 53 | 26.831 | 44.875 | 32.628 | 1.00 26.56 | CPS6 |
| MOTA | 5086 | CD | ARG | 53 | 27.406 | 43.749 | 31.834 | 1.00 28.57 | CPS6 |
| MOTA | 5087 | NE | ARG | 53 | 27.764 | 44.164 | 30.483 | 1.00 32.59 | CPS6 |
| ATOM | 5088 | CZ | ARG | 53 | 26.903 | 44.301 | 29.481 | 1.00 32.51 | CPS6 |
| ATOM | 5089 | NHl | ARG | 53 | 25.606 | 44.053 | 29.676 | 1.00 29.51 | CPS6 |
| MOTA | 5090 | NH2 | ARG | 53 | 27.352 | 44.666 | 28.277 | 1.00 29.31 | CPS6 |
| MOTA | 5091 | С | ARG | 53 | 27.081 | 42.951 | 35.926 | 1.00 22.03 | CPS6 |
| ATOM | 5092 | Ö | ARG | 53 | 28.014 | 42.159 | 35.983 | 1.00 22.12 | CPS6 |
| ATOM | 5093 | N | PHE | 54 | 26.576 | 43.541 | 37.000 | 1.00 20.72 | CPS6 |
| ATOM | 5094 | CA | PHE | 54 | 27.089 | 43.253 | 38.322 | 1.00 21.84 | CPS6 |
| ATOM | 5095 | CB | PHE | 54 | 26.391 | 44.144 | 39.347 | 1.00 23.57 | CPS6 |
| | | | | | | 43.925 | 40.756 | 1.00 24.76 | CPS6 |
| ATOM | 5096 | CG | PHE | 54 | 26.843 | | | | CPS6 |
| MOTA | 5097 | | PHE | 54 | 26.202 | 42.996 | 41.571 | 1.00 26.78 | |
| MOTA | 5098 | | PHE | 54 | 27.896 | 44.666 | 41.282 | 1.00 26.87 | CPS6 |
| MOTA | 5099 | CE1 | | 54 | 26.603 | 42.815 | 42.886 | 1.00 27.91 | CPS6 |
| ATOM | 5100 | CE2 | | 54 | 28.302 | 44.491 | 42.592 | 1.00 26.99 | CPS6 |
| MOTA | 5101 | CZ | PHE | 54 | 27.656 | 43.567 | 43.397 | 1.00 27.41 | CPS6 |
| MOTA | 5102 | C | PHE | 54 | 26.865 | 41.777 | 38.647 | 1.00 21.21 | CPS6 |
| ATOM | 5103 | 0 | PHE | 54 | 27.768 | 41.097 | 39.123 | 1.00 20.78 | CPS6 |
| ATOM | 5104 | N | ALA | 55 | 25.665 | 41.277 | 38.381 | 1.00 20.89 | CPS6 |
| MOTA | 5105 | CA | ALA | 55 | 25.374 | 39.872 | 38.669 | 1.00 20.22 | CPS6 |
| MOTA | 5106 | CB | ALA | 55 | 23.892 | 39.574 | 38.441 | 1.00 19.35 | CPS6 |
| ATOM | 5107 | C | ALA | 55 | 26.224 | 38.955 | 37.805 | 1.00 18.66 | CPS6 |
| ATOM | 5108 | 0 | ALA | 55 | 26.716 | 37.923 | 38.278 | 1.00 19.74 | CPS6 |
| ATOM | 5109 | N | ALA | 56 | 26.395 | 39.314 | 36.538 | 1.00 18.06 | CPS6 |
| ATOM | 5110 | CA | ALA | 56 | 27.195 | 38.488 | 35.639 | 1.00 18.21 | CPS6 |
| ATOM | 5111 | CB | ALA | 56 | 27.134 | 39.041 | 34.198 | 1.00 18.23 | CPS6 |
| | 5112 | C | ALA | 56 | 28.648 | 38.387 | 36.101 | 1.00 18.83 | CPS6 |
| ATOM | | | | 56 | 29.259 | 37.307 | 36.057 | 1.00 17.66 | CPS6 |
| MOTA | 5113 | 0 | ALA | | | 39.508 | 36.549 | 1.00 19.03 | CPS6 |
| MOTA | 5114 | N | LYS | 57 57 | 29.207 | | | 1.00 18.37 | CPS6 |
| ATOM | 5115 | CA | LYS | 57 | 30.592 | 39.513 | 37.012 | 1.00 18.37 | CPS6 |
| ATOM | 5116 | CB | LYS | 57 | 31.101 | 40.958 | 37.085 | | CPS6 |
| ATOM | 5117 | CG | LYS | 5 7 | 31.179 | 41.574 | 35.689 | 1.00 19.49 | |
| MOTA | 5118 | CD | LYS | 57 | 31.775 | 42.975 | 35.676 | 1.00 23.00 | CPS6 |
| MOTA | 5119 | CE | LYS | 57 | 31.663 | 43.579 | 34.285 | 1.00 20.60 | CPS6 |
| MOTA | 5120 | NZ | LYS | 57 | 32.580 | 44.729 | 34.103 | 1.00 21.27 | CPS6 |
| MOTA | 5121 | C | LYS | 57 | 30.745 | 38.785 | 38.344 | 1.00 19.47 | CPS6 |
| MOTA | 5122 | 0 | LYS | 57 | 31.739 | 38.084 | 38.557 | 1.00 20.88 | CPS6 |
| ATOM | 5123 | N | GLU | 58 | 29.773 | 38.942 | 39.245 | 1.00 19.43 | CPS6 |
| ATOM | 5124 | CA | GLU | 58 | 29.821 | 38.212 | 40.512 | 1.00 21.77 | CPS6 |
| ATOM | 5125 | CB | GLU | 58 | 28.640 | 38.591 | 41.419 | 1.00 22.85 | CPS6 |
| MOTA | 5126 | CG | GLU | 58 | 28.746 | 39.965 | 42.066 | 1.00 27.74 | CPS6 |
| ATOM | 5127 | CD | GLU | 58 | 29.884 | 40.060 | 43.079 | 1.00 30.88 | CPS6 |
| | | | | | | 41.173 | 43.580 | 1.00 34.74 | CPS6 |
| ATOM | 5128 | | GLU | 58 58 | 30.148 | | 43.378 | 1.00 34.71 | CPS6 |
| ATOM | 5129 | OE2 | GLU | 58 | 30.517 | 39.028 | 43.3/0 | 1.00 34.30 | C120 |

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| MOTA | 5130 | С | GLU | 58 | 29.745 | 36.711 | 40.199 | 1.00 21.81 | CPS6 |
|------|------|---------|-----|-----|--------|----------------|--------|------------|--------------|
| MOTA | 5131 | 0 | GLU | 58 | 30.494 | 35.900 | 40.767 | 1.00 21.58 | CPS6 |
| MOTA | 5132 | N | ALA | 59 | 28.833 | 36.332 | 39.305 | 1.00 20.31 | CPS6 |
| ATOM | 5133 | CA | ALA | 59 | 28.704 | 34.917 | 38.958 | 1.00 20.01 | CPS6 |
| ATOM | 5134 | CB | ALA | 59 | 27.557 | 34.709 | 37.956 | 1.00 19.39 | CPS6 |
| ATOM | 5135 | С | ALA | 59 | 30.015 | 34.398 | 38.370 | 1.00 20.62 | CPS6 |
| ATOM | 5136 | 0 | ALA | 59 | 30.463 | 33.289 | 38.693 | 1.00 21.08 | CPS6 |
| ATOM | 5137 | N | PHE | 60 | 30.625 | 35.192 | 37.497 | 1.00 18.52 | CPS6 |
| ATOM | 5138 | CA | PHE | 60 | 31.886 | 34.784 | 36.891 | 1.00 20.21 | CPS6 |
| ATOM | 5139 | CB | PHE | 60 | 32.359 | 35.819 | 35.863 | 1.00 19.79 | CPS6 |
| ATOM | 5140 | CG | PHE | 60 | 33.690 | 35.482 | 35.248 | 1.00 21.99 | CPS6 |
| ATOM | 5141 | CD1 | | 60 | 33.768 | 34.653 | 34.133 | 1.00 19.74 | CPS6 |
| ATOM | 5142 | CD2 | | 60 | 34.874 | 35.925 | 35.842 | 1.00 22.16 | CPS6 |
| ATOM | 5143 | | PHE | 60 | 35.010 | 34.264 | 33.618 | 1.00 23.98 | CPS6 |
| MOTA | 5144 | | PHE | 60 | 36.117 | 35.542 | 35.339 | 1.00 23.86 | CPS6 |
| ATOM | 5145 | CZ | PHE | 60 | 36.187 | 34.709 | 34.227 | 1.00 23.24 | CPS6 |
| ATOM | 5146 | C | PHE | 60 | 32.970 | 34.614 | 37.961 | 1.00 21.37 | CPS6 |
| ATOM | 5147 | 0 | PHE | 60 | 33.724 | 33.638 | 37.938 | 1.00 22.00 | CPS6 |
| ATOM | 5148 | N | SER | 61 | 33.048 | 35.565 | 38.891 | 1.00 21.71 | CPS6 |
| ATOM | 5149 | CA | SER | 61 | 34.065 | 35.516 | 39.945 | 1.00 21.71 | * |
| ATOM | 5150 | CB | SER | 61 | 34.003 | 36.772 | | 1.00 23.80 | CPS6 CPS6 |
| ATOM | | | | | | | 40.824 | | |
| | 5151 | OG G | SER | 61 | 32.938 | 36.694 | 41.753 | 1.00 25.60 | CPS6 |
| ATOM | 5152 | C | SER | 61 | 33.912 | 34.284 | 40.824 | 1.00 24.14 | CPS6 |
| ATOM | 5153 | 0 | SER | 61 | 34.897 | 33.786 | 41.386 | 1.00 25.44 | CPS6 |
| ATOM | 5154 | N | LYS | 62 | 32.683 | 33.800 | 40.957 | 1.00 23.98 | CPS6 |
| ATOM | 5155 | CA | LYS | 62 | 32.425 | 32.609 | 41.764 | 1.00 25.63 | CPS6 |
| MOTA | 5156 | CB | LYS | 62 | 30.946 | 32.566 | 42.174 | 1.00 25.79 | CPS6 |
| MOTA | 5157 | CG | LYS | 62 | 30.601 | 33.735 | 43.097 | 1.00 29.14 | CPS6 |
| MOTA | 5158 | CD | LYS | 62 | 29.112 | 33.966 | 43.281 | 1.00 32.29 | CPS6 |
| MOTA | 5159 | CE | LYS | 62 | 28.492 | 32.995 | 44.255 | 1.00 34.95 | CPS6 |
| MOTA | 5160 | NZ | LYS | 62 | 27.224 | 33.584 | 44.793 | 1.00 38.32 | CPS6 |
| ATOM | 5161 | C | LYS | 62 | 32.830 | 31.358 | 40.995 | 1.00 26.22 | CPS6 |
| ATOM | 5162 | 0 | LYS | 62 | 33.397 | 30.424 | 41.568 | 1.00 25.89 | CPS6 |
| ATOM | 5163 | N | ALA | 63 | 32.556 | 31.343 | 39.693 | 1.00 24.67 | CPS6 |
| MOTA | 5164 | CA | ALA | 63 | 32.936 | 30.209 | 38.861 | 1.00 24.83 | CPS6 |
| ATOM | 5165 | CB | ALA | 63 | 32.345 | 30.359 | 37.464 | 1.00 24.34 | CPS6 |
| ATOM | 5166 | C | ALA | 63 | 34.459 | 30.174 | 38.780 | 1.00 26.66 | CPS6 |
| ATOM | 5167 | 0 | ALA | 63 | 35.064 | 29.105 | 38.737 | 1.00 26.11 | CPS6 |
| ATOM | 5168 | N | PHE | 64 | 35.071 | 31.354 | 38.762 | 1.00 26.12 | CPS6 |
| ATOM | 5169 | CA | PHE | 64 | 36.526 | 31.467 | 38.692 | 1.00 28.50 | CPS6 |
| ATOM | 5170 | CB | PHE | 64 | 36.919 | 32.925 | 38.445 | 1.00 28.06 | CPS6 |
| MOTA | 5171 | CG | PHE | 64 | 38.341 | 33.104 | 37.992 | 1.00 29.52 | CPS6 |
| MOTA | 5172 | CD1 | PHE | 64 | 38.760 | 32.606 | 36.765 | 1.00 29.61 | CPS6 |
| MOTA | 5173 | CD2 | PHE | 64 | 39.251 | 33.787 | 38.787 | 1.00 29.01 | CPS6 |
| MOTA | 5174 | CEl | PHE | 64 | 40.072 | 32.787 | 36.329 | 1.00 32.11 | CPS6 |
| MOTA | 5175 | CE2 | PHE | 64 | 40.565 | 33.973 | 38.362 | 1.00 30.85 | CPS6 |
| MOTA | 5176 | CZ | PHE | 64 | 40.975 | 33,473 | 37.130 | 1.00 31.27 | CPS6 |
| ATOM | 5177 | С | PHE | 64 | 37.176 | 30.953 | 39.981 | 1.00 29.90 | CPS6 |
| ATOM | 5178 | 0 | PHE | 64 | 38.376 | 30.661 | 40.003 | 1.00 30.91 | CPS6 |
| ATOM | 5179 | N | GLY | 65 | 36.377 | 30.858 | 41.043 | 1.00 31.52 | CPS6 |
| ATOM | 5180 | CA | GLY | 65 | 36.845 | 30.349 | 42.322 | 1.00 34.23 | CPS6 |
| ATOM | 5181 | C | GLY | 65 | 37.435 | 31.337 | 43.315 | 1.00 36.45 | CPS6 |
| ATOM | 5182 | o | GLY | 65 | 37.726 | 30.968 | 44.456 | 1.00 37.62 | CPS6 |
| ATOM | 5183 | N | THR | 66 | 37.593 | 32.592 | 42.902 | 1.00 36.65 | CPS6 |
| ATOM | 5184 | CA | THR | 66 | 38.195 | 33.616 | 43.755 | 1.00 36.52 | CPS6 |
| ATOM | 5185 | CB | THR | 66 | 39.272 | 34.385 | 42.978 | 1.00 36.52 | CPS6 |
| MOTA | 5186 | | THR | 66 | 38.648 | 35.112 | 41.908 | 1.00 36.34 | CPS6 |
| ALON | 2200 | - J-G-I | | J J | 20.040 | J J . 4. 4. 4. | -1.700 | | |

| MOTA | 5187 | CG2 | THR | 66 | 40.297 | 33.429 | 42.389 | 1.00 36.79 | CPS6 |
|--------------|------------------------------|----------|------------|----------|------------------|------------------|--------|--------------------------|--------------|
| MOTA | 5188 | C | THR | 66 | 37.243 | 34.666 | 44.329 | 1.00 36.19 | CPS6 |
| MOTA | 5189 | 0 | THR | 66 | 37.475 | 35.193 | 45.419 | 1.00 35.77 | CPS6 |
| MOTA | 5190 | N | GLY | 67 | 36.175 | 34.973 | 43.599 | 1.00 35.09 | CPS6 |
| MOTA | 5191 | CA | GLY | 67 | 35.266 | 36.011 | 44.046 | 1.00 33.07 | CPS6 |
| MOTA | 5192 | С | GLY | 67 | 35.944 | 37.308 | 43.634 | 1.00 32.90 | CPS6 |
| ATOM | 5193 | 0 | GLY | 67 | 37.083 | 37.269 | 43.168 | 1.00 32.07 | CPS6 |
| ATOM | 5194 | N | ILE | 68 | 35.264 | 38.446 | 43.766 | 1.00 32.48 | CPS6 |
| ATOM | 5195 | CA | ILE | 68 | 35.878 | 39.721 | 43.397 | 1.00 32.14 | CPS6 |
| ATOM | 5196 | CB | ILE | 68 | 34.821 | 40.823 | 43.170 | 1.00 31.75 | CPS6 |
| ATOM | 5197 | CG2 | ILE | 68 | 35.509 | 42.167 | 42.928 | 1.00 32.21 | CPS6 |
| ATOM | 5198 | CG1 | ILE | 68 | 33.941 | 40.463 | 41.967 | 1.00 30.11 | CPS6 |
| ATOM | 5199 | CD1 | ILE | 68 | 34.697 | 40.354 | 40.642 | 1.00 30.32 | CPS6 |
| ATOM | 5200 | С | ILE | 68 | 36.796 | 40.150 | 44.536 | 1.00 33.67 | CPS6 |
| ATOM | 5201 | 0 | ILE | 68 | 36.370 | 40.206 | 45.692 | 1.00 33.24 | CPS6 |
| ATOM | 5202 | N | GLY | 69 | 38.050 | 40.443 | 44.207 | 1.00 34.42 | CPS6 |
| ATOM | 5203 | CA | GLY | 69 | 39.002 | 40.845 | 45.226 | 1.00 37.25 | CPS6 |
| MOTA | 5204 | С | GLY | 69 | 40.431 | 40.946 | 44.719 | 1.00 38.28 | CPS6 |
| MOTA | 5205 | 0 | GLY | 69 | 40.669 | 41.302 | 43.567 | 1.00 38.30 | CPS6 |
| MOTA | 5206 | N | ALA | 70 | 41.386 | 40.609 | 45.579 | 1.00 38.96 | CPS6 |
| MOTA | 5207 | CA | ALA | 70 | 42.800 | 40.684 | 45.233 | 1.00 39.69 | CPS6 |
| ATOM | 5208 | CB | ALA | 70 | 43.644 | 40.198 | 46.415 | 1.00 40.64 | CPS6 |
| ATOM | 5209 | C | ALA | 70 | 43.208 | 39.939 | 43.965 | 1.00 39.83 | CPS6 |
| ATOM | 5210 | 0 | ALA | 70 | 44.175 | 40.322 | 43.311 | 1.00 40.54 | CPS6 |
| ATOM | 5211 | N | GLN | 71 | 42.481 | 38.885 | 43.605 | 1.00 39.94 | CPS6 |
| MOTA | 5212 | CA | GLN | 71 | 42.834 | 38.115 | 42.411 | 1.00 39.34 | CPS6 |
| ATOM | 5213 | CB | GLN | 71 | 42.773 | 36.614 | 42.709 | 1.00 41.56 | CPS6 |
| ATOM | 5214 | CG | GLN | 71 | 43.429 | 36.181 | 44.006 | 1.00 43.98 | CPS6 |
| ATOM | 5215 | CD | GLN | 71 | 43.299 | 34.684 | 44.233 | 1.00 45.96 | CPS6 |
| ATOM | 5216 | | GLN | 71 | 43.901 | 33.880 | 43.515 | 1.00 48.14 | CPS6 |
| MOTA | 5217 | NE2 | GLN | 71 | 42.502 | 34.302 | 45.224 | 1.00 46.92 | CPS6 |
| MOTA | 5218 | C | GLN | 71 | 41.972 | 38.381 | 41.176 | 1.00 37.54 | CPS6 |
| ATOM | 5219 | 0 | GLN | 71 | 42.286 | 37.886 | 40.096 | 1.00 37.40 | CPS6 |
| ATOM | 5220 | N | LEU | 72 | 40.898 | 39.154 | 41.326 | 1.00 35.40 | CPS6 |
| ATOM | 5221 | CA | LEU | 72 | 39.998 | 39.428 | 40.204 | 1.00 33.24 | CPS6 |
| ATOM | 5222 | CB | LEU | 72 | 39.029 | 38.257 | 40.026 | 1.00 31.49 | CPS6 |
| ATOM | 5223 | CG | LEU | 72 | 38.647 | 37.600 | 38.692 | 1.00 32.42 1.00 28.80 | CPS6 |
| ATOM | 5224 | | | 72 | 37.168 | 37.243 | 38.788 | 1.00 28.80 | CPS6 |
| ATOM | 5225 | | LEU | 72 | 38.919 | 38.478 | 37.487 | 1.00 30.34 | CPS6 CPS6 |
| ATOM | 5226 | C | LEU LEU | 72 72 | 39.174 | 40.680 | 40.483 | 1.00 31.78 | CPS6 |
| ATOM | 5227 | 0 | | | 38.496 | 40.758 | 41.502 | 1.00 32.34 | CPS6 |
| ATOM | 5228 | N | SER | 73 73 | 39.217 38.428 | 41.652 42.866 | 39.784 | 1.00 30.83 | CPS6 |
| ATOM ATOM | 5229 | CA | SER | 73 73 | 39.289 | 44.113 | 39.615 | 1.00 29.35 | CPS6 |
| | 5230 5231 | CB | SER SER | 73 73 | 39.289 | 44.113 | 38.246 | 1.00 30.31 | CPS6 |
| MOTA | 523 2 | OG | SER | 73 73 | 37.309 | 42.898 | 38.752 | 1.00 30.23 | CPS6 |
| ATOM ATOM | 5232 | С О | SER | 73 73 | 37.333 | 42.147 | 37.775 | 1.00 27.49 | CPS6 |
| | 5234 | | PHE | 74 | 36.322 | 43.760 | 38.975 | 1.00 27.49 | CPS6 |
| ATOM | | N | | | | | 38.034 | 1.00 26.21 | CPS6 |
| MOTA MOTA | 523 5 523 6 | CA CB | PHE PHE | 74 74 | 35.213 34.219 | 43.888 | 38.534 | 1.00 25.21 | CPS6 |
| ATOM | 5236 | CG | PHE | 74 | 33.366 | 44.472 | 39.676 | 1.00 25.45 | CPS6 |
| ATOM | 5238 | | PHE | 74 | 32.329 | 43.568 | 39.460 | 1.00 27.07 | CPS6 |
| ATOM | 5239 | | PHE | 74 | 33.582 | 44.949 | 40.967 | 1.00 27.57 | CPS6 |
| ATOM | 5240 | | PHE | 74 | 31.511 | 43.148 | 40.515 | 1.00 27.84 | CPS6 |
| ATOM | 5241 | | PHE | 74 | 32.770 | 44.534 | 42.030 | 1.00 28.92 | CPS6 |
| ATOM | 5241 | CEZ | PHE | 74 | 31.732 | 43.634 | 41.801 | 1.00 27.85 | CPS6 |
| ATOM | 5242 | C | PHE | 74 | 35.731 | 44.301 | 36.659 | 1.00 26.17 | CPS6 |
| 7100 | 2243 | _ | | , - | 22.721 | 11.501 | 55.055 | | |

| MOTA | 5244 | 0 | PHE | 74 | 35.186 | 43.903 | 35.638 | 1.00 25.99 | CPS6 |
|--------------|--------------|---------|------------|------------------|------------------|------------------|------------------|------------|--------------|
| ATOM | 5245 | N | GLN | 75 | 36.793 | 45.103 | 36.638 | 1.00 25.96 | CPS6 |
| ATOM | 5246 | CA | GLN | 75 | 37.365 | 45.583 | 35.384 | 1.00 27.32 | CPS6 |
| ATOM | 5247 | CB | GLN | 75 | 38.374 | 46.703 | 35.665 | 1.00 27.52 | CPS6 |
| MOTA | 5248 | CG | GLN | 75 | 37.754 | 47.960 | 36.271 | 1.00 30.15 | CPS6 |
| ATOM | 5249 | CD | GLN | 75 | 36.770 | 48.648 | 35.339 | 1.00 30.80 | CPS6 |
| ATOM | 5250 | OF1 | GLN | 75 | 37.052 | 48.857 | 34.159 | 1.00 31.37 | CPS6 |
| MOTA | 5251 | NE2 | GLN | 75 | 35.618 | 49.019 | 35.871 | 1.00 34.02 | CPS6 |
| MOTA | 5252 | C | GLN | 75 | 38.024 | 44.498 | 34.530 | 1.00 26.97 | CPS6 |
| MOTA | 5253 | 0 | GLN | 75 | 38.199 | 44.679 | 33.329 | 1.00 26.86 | CPS6 |
| MOTA | 5254 | N | ASP | 76 | 38.382 | 43.377 | 35.150 | 1.00 27.98 | CPS6 |
| ATOM | 5255 | CA | ASP | 76 | 39.004 | 42.258 | 34.437 | 1.00 27.78 | CPS6 |
| MOTA | 5256 | CB | ASP | 76 | 39.644 | 41.271 | 35.421 | 1.00 29.90 | CPS6 |
| ATOM | 5257 | CG | ASP | 76 | 40.883 | 41.813 | 36.091 | 1.00 31.18 | CPS6 |
| ATOM | 5258 | OD1 | ASP | 76 | 41.690 | 42.457 | 35.397 | 1.00 35.07 | CPS6 |
| ATOM | 5259 | OD2 | ASP | 76 | 41.059 | 41.570 | 37.307 | 1.00 32.81 | CPS6 |
| ATOM | 5260 | C | ASP | 76 | 37.969 | 41.474 | 33.633 | 1.00 27.27 | CPS6 |
| MOTA | 5261 | 0 | ASP | 76 | 38.314 | 40.671 | 32.764 | 1.00 26.16 | CPS6 |
| MOTA | 5262 | N | ILE | 77 | 36.696 | 41.705 | 33.930 | 1.00 26.25 | CPS6 |
| MOTA | 5263 | CA | ILE | 77 | 35.616 | 40.966 | 33.272 | 1.00 25.67 | CPS6 |
| MOTA | 5264 | CB | ILE | 77 | 34.682 | 40.360 | 34.335 | 1.00 25.40 | CPS6 |
| ATOM | 5265 | CG2 | ILE | 77 | 33.688 | 39.404 | 33.681 | 1.00 24.95 | CPS6 |
| ATOM | 5266 | CG1 | ILE | 77 | 35.511 | 39.639 | 35.400 | 1.00 23.36 | CPS6 |
| ATOM | 5267 | CD1 | ILE | 77 | 34.798 | 39.549 | 36.758 | 1.00 23.84 | CPS6 |
| ATOM | 5268 | С | ILE | 77 | 34.785 | 41.871 | 32.372 | 1.00 25.23 | CPS6 |
| ATOM | 5269 | 0 | ILE | 7 7 | 34.326 | 42.916 | 32.809 | 1.00 26.66 | CPS6 |
| ATOM | 5270 | N | GLU | 78 | 34.579 | 41.473 | 31.123 | 1.00 24.36 | CPS6 |
| ATOM | 5271 | CA | GLU | 78 | 33.794 | 42.296 | 30.217 | 1.00 23.95 | CPS6 |
| ATOM | 5272 | CB | GLU | 78 | 34.689 | 42.928 | 29.151 | 1.00 23.23 | CPS6 |
| ATOM | 5273 | CG | GLU | 78 | 33.936 | 43.867 | 28.231 | 1.00 25.47 | CPS6 |
| ATOM | 5274 | CD | GLU | 78 | 34.858 | 44.740 | 27.406 | 1.00 28.41 | CPS6 |
| ATOM | 5275 | | GLU | 78 | 35.313 | 44.287 | 26.331 | 1.00 28.29 | CPS6 |
| MOTA | 5276 | OE2 | | 78 | 35.133 | 45.880 | 27.844 | 1.00 29.93 | CPS6 |
| MOTA | 5277 | C | GLU | 78 | 32.698 | 41.501 | 29.523 | 1.00 23.31 | CPS6 |
| ATOM | 5278 | 0 | GLU | 78 | 32.951 | 40.411 | 29.013 | 1.00 23.66 | CPS6 |
| ATOM | 5279 | N | ILE | 79 70 | 31.481 | 42.045 | 29.519 | 1.00 23.40 | CPS6 |
| ATOM | 5280 | CA | ILE | 79 7 0 | 30.376 | 41.377 | 28.843 | 1.00 22.82 | CPS6 CPS6 |
| ATOM | 5281 | CB | ILE | 79 | 29.074 | 41.348 | 29.696 | 1.00 22.78 | CPS6 |
| ATOM | 5282 | CG2 | | 79 70 | 27.899 | 40.913 | 28.834 | 1.00 23.83 | CPS6 |
| ATOM | 5283 | CG1 | | 79 79 | 29.214 | 40.370 | 30.871 | 1.00 25.82 | CPS6 |
| ATOM | 5284 | CDI | ILE | 79 79 | 29.978 30.081 | 40.908 | 32.041 27.551 | 1.00 28.29 | CPS6 |
| ATOM | 5285 | | | 79 79 | 29.992 | 42.125 43.352 | 27.531 | 1.00 22.39 | CPS6 |
| ATOM | 5286 5287 | 0 | ILE | 80 | 29.969 | 41.383 | 26.456 | 1.00 22.11 | CPS6 |
| MOTA MOTA | 5288 | N CA | ARG ARG | 80 | 29.625 | 41.363 | 25.152 | 1.00 24.89 | CPS6 |
| ATOM | 5289 | CB | ARG | 80 | 30.781 | 41.821 | 24.147 | 1.00 28.30 | CPS6 |
| ATOM | 5290 | CG | ARG | 80 | 32.171 | 41.662 | 24.758 | 1.00 34.49 | CPS6 |
| ATOM | 5291 | CD | ARG | 80 | 33.065 | 42.894 | 24.630 | 1.00 37.92 | CPS6 |
| ATOM | 5292 | NE | ARG | 80 | 33.175 | 43.397 | 23.267 | 1.00 39.97 | CPS6 |
| ATOM | 5292 | CZ | ARG | 80 | 34.078 | 44.291 | 22.857 | 1.00 39.55 | CPS6 |
| ATOM | 5294 | | ARG | 80 | 34.078 | 44.787 | 23.697 | 1.00 38.56 | CPS6 |
| ATOM | 5295 | | ARG | 80 | 34.050 | 44.724 | 21.604 | 1.00 37.96 | CPS6 |
| ATOM | 5296 | C | ARG | 80 | 28.445 | 41.119 | 24.657 | 1.00 24.70 | CPS6 |
| MOTA | 5297 | 0 | ARG | 80 | 28.130 | 40.095 | 25.249 | 1.00 22.24 | CPS6 |
| MOTA | 5298 | Ŋ | LYS | 81 | 27.776 | 41.551 | 23.592 | 1.00 26.22 | CPS6 |
| MOTA | 5299 | CA | LYS | 81 | 26.664 | 40.770 | 23.055 | 1.00 28.06 | CPS6 |
| MOTA | 5300 | CB | LYS | 81 | 25.346 | 41.547 | 23.140 | 1.00 30.47 | CPS6 |
| ALUM | 2200 | | | - | 22.240 | | | | |

| ATOM | 5301 | CG | LYS | 81 | 24.745 | 41.614 | 24.542 | 1.00 34.14 | CPS6 |
|------|------|-----|-----|----|--------|--------|--------|------------|------|
| ATOM | 5302 | CD | LYS | 81 | 23.460 | 42.439 | 24.545 | 1.00 37.71 | CPS6 |
| ATOM | 5303 | CE | LYS | 81 | 22.985 | 42.787 | 25.963 | 1.00 37.71 | |
| | | | | | | | | | CPS6 |
| ATOM | 5304 | NZ | LYS | 81 | 22.435 | 41.636 | 26.736 | 1.00 39.75 | CPS6 |
| MOTA | 5305 | C | LYS | 81 | 26.962 | 40.409 | 21.608 | 1.00 29.13 | CPS6 |
| MOTA | 5306 | 0 | LYS | 81 | 27.536 | 41.222 | 20.876 | 1.00 29.46 | CPS6 |
| MOTA | 5307 | N | ASP | 82 | 26.602 | 39.193 | 21.197 | 1.00 29.17 | CPS6 |
| MOTA | 5308 | CA | ASP | 82 | 26.861 | 38.783 | 19.824 | 1.00 31.09 | CPS6 |
| ATOM | 5309 | CB | ASP | 82 | 27.044 | 37.255 | 19.707 | 1.00 29.73 | CPS6 |
| MOTA | 5310 | CG | ASP | 82 | 25.751 | 36.464 | 19.877 | 1.00 28.91 | CPS6 |
| ATOM | 5311 | OD1 | ASP | 82 | 24.646 | 37.045 | 19.861 | 1.00 26.18 | CPS6 |
| ATOM | 5312 | OD2 | ASP | 82 | 25.861 | 35.226 | 20.012 | 1.00 28.29 | CPS6 |
| ATOM | 5313 | C | ASP | 82 | 25.775 | 39.283 | 18.891 | 1.00 31.70 | CPS6 |
| ATOM | 5314 | 0 | ASP | 82 | 24.909 | 40.051 | 19.306 | 1.00 32.19 | CPS6 |
| MOTA | 5314 | N | GLN | 83 | 25.821 | 38.852 | 17.634 | 1.00 35.43 | CPS6 |
| | | | | | | | | | CPS6 |
| ATOM | 5316 | CA | GLN | 83 | 24.854 | 39.300 | 16.634 | 1.00 37.80 | |
| ATOM | 5317 | CB | GLN | 83 | 25.222 | 38.738 | 15.252 | 1.00 40.89 | CPS6 |
| MOTA | 5318 | CG | GLN | 83 | 25.267 | 37.219 | 15.164 | 1.00 44.70 | CPS6 |
| MOTA | 5319 | CD | GLN | 83 | 26.534 | 36.612 | 15.755 | 1.00 47.79 | CPS6 |
| MOTA | 5320 | | GLN | 83 | 26.642 | 35.388 | 15.889 | 1.00 49.81 | CPS6 |
| MOTA | 5321 | NE2 | GLN | 83 | 27.503 | 37.461 | 16.101 | 1.00 48.69 | CPS6 |
| MOTA | 5322 | С | GLN | 83 | 23.400 | 38.966 | 16.965 | 1.00 38.04 | CPS6 |
| ATOM | 5323 | 0 | GLN | 83 | 22.481 | 39.641 | 16.499 | 1.00 38.72 | CPS6 |
| ATOM | 5324 | N | ASN | 84 | 23.182 | 37.933 | 17.772 | 1.00 36.73 | CPS6 |
| ATOM | 5325 | CA | ASN | 84 | 21.822 | 37.564 | 18.146 | 1.00 35.24 | CPS6 |
| MOTA | 5326 | CB | ASN | 84 | 21.701 | 36.049 | 18.292 | 1.00 35.98 | CPS6 |
| ATOM | 5327 | CG | ASN | 84 | 21.864 | 35.331 | 16.979 | 1.00 37.29 | CPS6 |
| ATOM | 5328 | | ASN | 84 | 21.242 | 35.699 | 15.977 | 1.00 39.43 | CPS6 |
| ATOM | 5329 | | ASN | 84 | 22.694 | 34.298 | 16.968 | 1.00 36.91 | CPS6 |
| ATOM | 5330 | C | ASN | 84 | 21.400 | 38.234 | 19.447 | 1.00 33.77 | CPS6 |
| ATOM | 5331 | 0 | ASN | 84 | 20.262 | 38.088 | 19.882 | 1.00 34.74 | CPS6 |
| MOTA | 5332 | N | GLY | 85 | 22.322 | 38.963 | 20.067 | 1.00 31.96 | CPS6 |
| | | | GLY | 85 | 22.011 | 39.635 | 21.315 | 1.00 30.32 | CPS6 |
| MOTA | 5333 | CA | | | | | | 1.00 30.32 | CPS6 |
| ATOM | 5334 | C | GLY | 85 | 22.360 | 38.777 | 22.520 | | CPS6 |
| MOTA | 5335 | 0 | GLY | 85 | 22.022 | 39.112 | 23.655 | 1.00 28.08 | |
| ATOM | 5336 | N | LYS | 86 | 23.041 | 37.664 | 22.265 | 1.00 26.87 | CPS6 |
| ATOM | 5337 | CA | LYS | 86 | 23.451 | 36.743 | 23.323 | 1.00 24.77 | CPS6 |
| MOTA | 5338 | CB | LYS | 86 | 23.760 | 35.365 | 22.719 | 1.00 24.34 | CPS6 |
| ATOM | 5339 | CG | LYS | 86 | 24.446 | 34.376 | 23.663 | 1.00 23.41 | CPS6 |
| ATOM | 5340 | CD | LYS | 86 | 23.518 | 33.886 | 24.783 | 1.00 22.54 | CPS6 |
| ATOM | 5341 | CE | LYS | 86 | 24.296 | 33.008 | 25.778 | 1.00 21.86 | CPS6 |
| MOTA | 5342 | NZ | LYS | 86 | 23.395 | 32.379 | 26.784 | 1.00 21.67 | CPS6 |
| ATOM | 5343 | C | LYS | 86 | 24.690 | 37.282 | 24.028 | 1.00 23.40 | CPS6 |
| ATOM | 5344 | 0 | LYS | 86 | 25.709 | 37.558 | 23.390 | 1.00 22.20 | CPS6 |
| ATOM | 5345 | N | PRO | 87 | 24.628 | 37.443 | 25.359 | 1.00 22.90 | CPS6 |
| MOTA | 5346 | CD | PRO | 87 | 23.483 | 37.328 | 26.283 | 1.00 23.21 | CPS6 |
| MOTA | 5347 | CA | PRO | 87 | 25.820 | 37.956 | 26.050 | 1.00 21.73 | CPS6 |
| MOTA | 5348 | CB | PRO | 87 | 25.281 | 38.351 | 27.427 | 1.00 23.57 | CPS6 |
| MOTA | 5349 | CG | PRO | 87 | 24.166 | 37.350 | 27.648 | 1.00 23.73 | CPS6 |
| | 5350 | C | PRO | 87 | 26.945 | 36.924 | 26.167 | 1.00 21.97 | CPS6 |
| ATOM | | | | 87 | 26.693 | 35.724 | 26.260 | 1.00 19.28 | CPS6 |
| ATOM | 5351 | 0 | PRO | | | | | 1.00 21.22 | CPS6 |
| ATOM | 5352 | N | TYR | 88 | 28.192 | 37.393 | 26.124 | 1.00 21.22 | CPS6 |
| ATOM | 5353 | CA | TYR | 88 | 29.333 | 36.504 | 26.308 | | |
| ATOM | 5354 | CB | TYR | 88 | 29.881 | 35.972 | 24.980 | 1.00 22.01 | CPS6 |
| ATOM | 5355 | CG | TYR | 88 | 30.434 | 37.009 | | 1.00 21.99 | CPS6 |
| ATOM | 5356 | | TYR | 88 | 31.796 | 37.317 | | 1.00 25.46 | CPS6 |
| ATOM | 5357 | CE1 | TYR | 88 | 32.310 | 38.251 | 23.121 | 1.00 24.59 | CPS6 |
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|------|--------------|-----|-----|-----|--------|--------|--------|------------|------|
| MOTA | 5358 | CD2 | TYR | 88 | 29.600 | 37.666 | 23.132 | 1.00 25.11 | CPS6 |
| MOTA | 5359 | CE2 | TYR | 83 | 30.105 | 38.601 | 22.234 | 1.00 25.50 | CPS6 |
| ATOM | 5360 | CZ | TYR | 88 | 31.459 | 38.887 | 22.235 | 1.00 26.13 | CPS6 |
| MOTA | 5361 | OH | TYR | 88 | 31.947 | 39.824 | 21.351 | 1.00 28.03 | CPS6 |
| ATOM | 5362 | С | TYR | 88 | 30.382 | 37.287 | 27.062 | 1.00 21.33 | CPS6 |
| ATOM | 5363 | ō | TYR | 88 | 30.415 | 38.512 | 27.009 | 1.00 22.02 | CPS6 |
| | | | | | | | | | |
| ATOM | 5364 | N | ILE | 89 | 31.238 | 36.571 | 27.769 | 1.00 22.15 | CPS6 |
| MOTA | 5365 | CA | ILE | 89 | 32.263 | 37.187 | 28.581 | 1.00 22.97 | CPS6 |
| MOTA | 5366 | CB | ILE | 89 | 32.244 | 36.555 | 30.001 | 1.00 22.83 | CPS6 |
| MOTA | 5367 | CG2 | ILE | 89 | 33.564 | 36.820 | 30.736 | 1.00 22.49 | CPS6 |
| MOTA | 5368 | CG1 | ILE | 89 | 31.036 | 37.080 | 30.779 | 1.00 23.07 | CPS6 |
| ATOM | 5369 | CD1 | ILE | 89 | 30.876 | 36.460 | 32.168 | 1.00 23.21 | CPS6 |
| | 5370 | | ILE | | 33.670 | 37.026 | 28.027 | 1.00 24.96 | CPS6 |
| ATOM | | C | | 89 | | | | | |
| MOTA | 5371 | 0 | ILE | 89 | 33.990 | 35.997 | 27.435 | 1.00 24.10 | CPS6 |
| ATOM | 5372 | N | ILE | 90 | 34.489 | 38.064 | 28.193 | 1.00 24.59 | CPS6 |
| MOTA | 5373 | CA | ILE | 90 | 35.898 | 37.956 | 27.833 | 1.00 25.62 | CPS6 |
| MOTA | 5374 | CB | ILE | 90 | 36.305 | 38.796 | 26.589 | 1.00 26.38 | CPS6 |
| MOTA | 5375 | CG2 | ILE | 90 | 35.630 | 38.229 | 25.360 | 1.00 26.74 | CPS6 |
| ATOM | 5376 | CG1 | ILE | 90 | 35.984 | 40.273 | 26.787 | 1.00 27.06 | CPS6 |
| ATOM | 5377 | CD1 | ILE | 90 | 36.410 | 41.147 | 25.584 | 1.00 30.06 | CPS6 |
| | | | | 90 | 36.657 | 38.407 | 29.079 | 1.00 26.15 | CPS6 |
| MOTA | 5378 | C | ILE | | | | | | |
| ATOM | 5379 | 0 | ILE | 90 | 36.241 | 39.337 | 29.783 | 1.00 25.40 | CPS6 |
| MOTA | 5380 | И | CYS | 91 | 37.742 | 37.702 | 29.376 | 1.00 26.82 | CPS6 |
| MOTA | 5381 | CA | CYS | 91 | 38.574 | 37.975 | 30.543 | 1.00 28.62 | CPS6 |
| MOTA | 5382 | CB | CYS | 91 | 38.041 | 37.191 | 31.749 | 1.00 27.71 | CPS6 |
| ATOM | 5383 | SG | CYS | 91 | 39.031 | 37.333 | 33.261 | 1.00 30.47 | CPS6 |
| MOTA | 5384 | C | CYS | 91 | 39.998 | 37.516 | 30.194 | 1.00 29.98 | CPS6 |
| MOTA | 5385 | ō | CYS | 91 | 40.213 | 36.361 | 29.839 | 1.00 29.65 | CPS6 |
| | 5386 | N | THR | 92 | 40.966 | 38.419 | 30.291 | 1.00 32.42 | CPS6 |
| ATOM | | | | | | | 29.948 | 1.00 34.14 | CPS6 |
| ATOM | 5387 | CA | THR | 92 | 42.344 | 38.078 | | | |
| MOTA | 5388 | CB | THR | 92 | 43.264 | 39.303 | 30.103 | 1.00 36.33 | CPS6 |
| ATOM | 5389 | 0G1 | | 92 | 43.150 | 39.810 | 31.439 | 1.00 38.35 | CPS6 |
| ATOM | 5390 | CG2 | THR | 92 | 42.872 | 40.393 | 29.104 | 1.00 35.90 | CPS6 |
| MOTA | 5391 | C | THR | 92 | 42.931 | 36.932 | 30.761 | 1.00 35.10 | CPS6 |
| ATOM | 5392 | 0 | THR | 92 | 43.960 | 36.359 | 30.380 | 1.00 36.58 | CPS6 |
| ATOM | 5393 | N | LYS | 93 | 42.291 | 36.582 | 31.870 | 1.00 33.97 | CPS6 |
| MOTA | 5394 | CA | LYS | 93 | 42.808 | 35.503 | 32.698 | 1.00 34.28 | CPS6 |
| ATOM | 5395 | CB | LYS | 93 | 42.231 | 35.596 | 34.105 | 1.00 35.19 | CPS6 |
| | | | | | | 36.867 | 34.827 | 1.00 38.98 | CPS6 |
| ATOM | 5396 | CG | LYS | 93 | 42.654 | | | 1.00 40.89 | CPS6 |
| MOTA | 5397 | CD | LYS | 93 | 42.107 | 36.924 | 36.240 | | |
| MOTA | 539 8 | CE | LYS | 93 | 42.416 | 38.263 | 36.898 | 1.00 41.92 | CPS6 |
| MOTA | 5399 | NZ | LYS | 93 | 43.879 | 38.529 | 36.966 | 1.00 43.76 | CPS6 |
| ATOM | 5400 | C | LYS | 93 | 42.575 | 34.111 | 32.126 | 1.00 33.08 | CPS6 |
| MOTA | 5401 | 0 | LYS | 93 | 43.143 | 33.137 | 32.613 | 1.00 33.58 | CPS6 |
| ATOM | 5402 | N | LEU | 94 | 41.743 | 34.005 | 31.098 | 1.00 31.56 | CPS6 |
| ATOM | 5403 | CA | LEU | 94 | 41.489 | 32.702 | 30.487 | 1.00 29.96 | CPS6 |
| | 5404 | CB | LEU | 94 | 40.553 | 31.853 | 31.363 | 1.00 31.34 | CPS6 |
| MOTA | | | | | 39.321 | | 32.035 | 1.00 33.01 | CPS6 |
| ATOM | 5405 | CG | LEU | 94 | | 32.481 | | 1.00 33.01 | CPS6 |
| MOTA | 5406 | | LEU | 94 | 38.520 | 33.306 | 31.062 | | |
| MOTA | 5407 | | LEU | 94 | 38.465 | 31.368 | 32.625 | 1.00 35.31 | CPS6 |
| ATOM | 5408 | C | LEU | 94 | 40.917 | 32.822 | 29.091 | 1.00 28.50 | CPS6 |
| ATOM | 5409 | 0 | LEU | 94 | 40.531 | 33.909 | 28.654 | 1.00 28.02 | CPS6 |
| ATOM | 5410 | N | SER | 95 | 40.861 | 31.692 | 28.398 | 1.00 27.95 | CPS6 |
| ATOM | 5411 | CA | SER | 95 | 40.341 | 31.636 | 27.040 | 1.00 27.87 | CPS6 |
| ATOM | 5412 | CB | SER | 95 | 40.579 | 30.261 | | 1.00 28.47 | CPS6 |
| | | | | | | | | 1.00 30.54 | CPS6 |
| MOTA | 5413 | OG | SER | 95 | 39.846 | 30.141 | | | CPS6 |
| ATOM | 5414 | C | SER | 95 | 38.849 | 31.905 | 27.011 | 1.00 20.00 | C230 |

| ATOM | 5415 | 0 | SER | 95 | 38.098 | 31.331 | 27.793 | 1.00 25.68 | CPS6 |
|------|--------------|-----|-------|-----|--------|--------|--------|------------|------|
| ATOM | 5416 | N | PRO | 96 | 38.401 | 32.762 | 26.082 | 1.00 25.92 | CPS6 |
| ATOM | 5417 | CD | PRO | 96 | 39.206 | 33.567 | 25.144 | 1.00 25.77 | CPS6 |
| ATOM | 5418 | CA | PRO | 96 | 36.978 | 33.085 | 25.978 | 1.00 25.00 | CPS6 |
| ATOM | 5419 | CB | PRO | 96 | 36.947 | 34.199 | 24.922 | 1.00 25.69 | CPS6 |
| ATOM | 5420 | CG | PRO | 96 | 38.197 | 33.949 | 24.093 | 1.00 25.08 | CPS6 |
| | | | | | | | | | |
| ATOM | 5421 | C | PRO | 96 | 36.129 | 31.873 | 25.602 | 1.00 25.28 | CPS6 |
| ATOM | 5422 | 0 | PRO | 96 | 34.942 | 31.810 | 25.922 | 1.00 23.78 | CPS6 |
| ATOM | 5423 | N | ALA | 97 | 36.741 | 30.902 | 24.934 | 1.00 24.13 | CPS6 |
| MOTA | 5424 | CA | ALA | 97 | 36.023 | 29.701 | 24.534 | 1.00 24.78 | CPS6 |
| MOTA | 5425 | CB | ALA | 97 | 36.873 | 28.890 | 23.569 | 1.00 25.54 | CPS6 |
| MOTA | 5426 | C | ALA | 97 | 35.650 | 28.846 | 25.746 | 1.00 24.39 | CPS6 |
| ATOM | 5427 | 0 | ALA | 97 | 34.783 | 27.980 | 25.657 | 1.00 25.77 | CPS6 |
| ATOM | 5428 | N | ALA | 98 | 36.300 | 29.093 | 26.879 | 1.00 23.13 | CPS6 |
| ATOM | 5429 | CA | ALA | 98 | 36.033 | 28.320 | 28.094 | 1.00 23.12 | CPS6 |
| ATOM | 5430 | CB | ALA | 98 | 37.285 | 28.277 | 28.947 | 1.00 23.94 | CPS6 |
| MOTA | 5431 | c | ALA | 98 | 34.875 | 28.867 | 28.937 | 1.00 23.29 | CPS6 |
| ATOM | 5432 | 0 | ALA | 98 | 34.418 | 28.217 | 29.883 | 1.00 23.78 | CPS6 |
| | | | VAL | 99 | 34.398 | 30.055 | 28.593 | 1.00 23.70 | CPS6 |
| ATOM | 5433 | N | | | | | 29.386 | 1.00 22.03 | CPS6 |
| ATOM | 5434 | CA | VAL | 99 | 33.353 | 30.693 | | | CPS6 |
| ATOM | 5435 | CB | VAL | 99 | 33.776 | 32.130 | 29.747 | 1.00 22.74 | |
| MOTA | 5436 | | VAL | 99 | 32.850 | 32.710 | 30.799 | 1.00 22.51 | CPS6 |
| MOTA | 5437 | | VAL | 99 | 35.207 | 32.132 | 30.250 | 1.00 24.89 | CPS6 |
| MOTA | 5438 | C | LAV | 99 | 31.978 | 30.757 | 28.739 | 1.00 20.85 | CPS6 |
| ATOM | 5439 | 0 | VAL | 99 | 31.850 | 30.969 | 27.534 | 1.00 20.38 | CPS6 |
| ATOM | 5440 | N | HIS | 100 | 30.950 | 30.580 | 29.568 | 1.00 20.29 | CPS6 |
| ATOM | 5441 | CA | HIS | 100 | 29.563 | 30.652 | 29.132 | 1.00 18.65 | CPS6 |
| ATOM | 5442 | CB | HIS | 100 | 28.988 | 29.251 | 29.029 | 1.00 20.06 | CPS6 |
| MOTA | 5443 | CG | HIS | 100 | 29.786 | 28.360 | 28.139 | 1.00 23.66 | CPS6 |
| MOTA | 5444 | CD2 | HIS | 100 | 30.802 | 27.509 | 28.412 | 1.00 26.19 | CPS6 |
| ATOM | 5445 | ND1 | HIS | 100 | 29.626 | 28.343 | 26.772 | 1.00 25.30 | CPS6 |
| ATOM | 5446 | | HIS | 100 | 30.511 | 27.518 | 26.239 | 1.00 26.78 | CPS6 |
| ATOM | 5447 | | HIS | 100 | 31.237 | 27.000 | 27.214 | 1.00 27.25 | CPS6 |
| ATOM | 5448 | C | HIS | 100 | 28.806 | 31.440 | 30.186 | 1.00 18.48 | CPS6 |
| MOTA | 5449 | o | HIS | 100 | 29.071 | 31.297 | 31.378 | 1.00 17.96 | CPS6 |
| MOTA | 5450 | И | VAL | 101 | 27.852 | 32.261 | 29.753 | 1.00 17.67 | CPS6 |
| | | CA | VAL | 101 | 27.092 | 33.060 | 30.697 | 1.00 17.87 | CPS6 |
| ATOM | 5451 | | VAL | | 27.749 | 34.455 | 30.846 | 1.00 17.07 | CPS6 |
| ATOM | 5452 | CB | | 101 | | | 29.492 | 1.00 19.75 | CPS6 |
| MOTA | 5453 | | VAL | 101 | 27.766 | | | 1.00 19.73 | CPS6 |
| ATOM | 5454 | | VAL | 101 | 26.984 | 35.314 | 31.860 | | CPS6 |
| MOTA | 5455 | С | VAL | 101 | 25.650 | 33.255 | 30.229 | 1.00 17.14 | CPS6 |
| MOTA | 5456 | 0 | VAL | 101 | 25.356 | 33.139 | 29.046 | 1.00 16.92 | |
| MOTA | 545 7 | N | SER | 102 | | 33.522 | 31.173 | | CPS6 |
| ATOM | 5458 | CA | SER | 102 | 23.365 | 33.821 | 30.837 | 1.00 18.24 | CPS6 |
| ATOM | 5459 | CB | SER | 102 | 22.450 | 32.592 | 30.926 | 1.00 18.94 | CPS6 |
| MOTA | 5460 | OG | SER | 102 | 21.131 | 32.955 | 30.513 | 1.00 19.02 | CPS6 |
| MOTA | 5461 | C | SER | 102 | 22.932 | 34.853 | 31.855 | 1.00 17.95 | CPS6 |
| MOTA | 5462 | 0 | SER | 102 | 23.335 | 34.792 | 33.025 | 1.00 16.39 | CPS6 |
| ATOM | 5463 | N | ILE | 103 | 22.112 | | 31.414 | 1.00 16.51 | CPS6 |
| ATOM | 5464 | CA | ILE | 103 | 21.630 | 36.864 | | 1.00 17.17 | CPS6 |
| ATOM | 5465 | CB | ILE | 103 | 22.243 | | | 1.00 17.60 | CPS6 |
| ATOM | 5466 | | ILE | 103 | 21.761 | | | 1.00 19.81 | CPS6 |
| | | | ILE | 103 | 23.769 | | | 1.00 19.89 | CPS6 |
| ATOM | 5467 | | | | | | | | CPS6 |
| ATOM | 5468 | | . ILE | 103 | 24.483 | | | 1.00 17.69 | CPS6 |
| MOTA | 5469 | C | ILE | 103 | 20.112 | | | | CPS6 |
| ATOM | 5470 | 0 | ILE | 103 | 19.595 | | | | CPS6 |
| MOTA | 5471 | N | THR | 104 | 19.414 | 37.173 | 33.237 | 1.00 18.18 | Crob |
| | | | | | | | | | |

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| ATOM | 5472 | CA | THR | 104 | 17.954 | 37.283 | 33.226 | 1.00 18.92 | CPS6 |
|--------------|--------------|-----|-----|-----|------------------|--------|------------------|------------|------|
| ATOM | 5473 | CB | THR | 104 | 17.285 | 35.948 | 33.660 | 1.00 20.47 | CPS6 |
| MOTA | 5474 | OG1 | THR | 104 | 15.864 | 36.026 | 33.456 | 1.00 20.23 | CPS6 |
| ATOM | 5475 | CG2 | THR | 104 | 17.578 | 35.648 | 35.130 | 1.00 17.86 | CPS6 |
| MOTA | 5476 | C | THR | 104 | 17.523 | 38.429 | 34.159 | 1.00 20.41 | CPS6 |
| MOTA | 5477 | 0 | THR | 104 | 18.306 | 38.901 | 34.990 | 1.00 19.19 | CPS6 |
| ATOM | 5478 | N | HIS | 105 | 16.280 | 38.880 | 34.001 | 1.00 21.31 | CPS6 |
| ATOM | 5479 | CA | HIS | 105 | 15.751 | 39.984 | 34.799 | 1.00 22.86 | CPS6 |
| MOTA | 5480 | CB | HIS | 105 | 15.802 | 41.299 | 33.998 | 1.00 26.24 | CPS6 |
| ATOM | 5481 | CG | HIS | 105 | 17.175 | 41.721 | 33.578 | 1.00 30.59 | CPS6 |
| ATOM | 5482 | | HIS | 105 | 17.889 | 41.444 | 32.461 | 1.00 32.14 | CPS6 |
| ATOM | 5483 | ND1 | | 105 | 17.974 | 42.534 | 34.355 | 1.00 33.04 | CPS6 |
| ATOM | 5484 | | HIS | 105 | 19.122 | 42.739 | 33.733 | 1.00 33.19 | CPS6 |
| ATOM | 5485 | NE2 | | 105 | 19.097 | 42.089 | 32.582 | 1.00 32.49 | CPS6 |
| MOTA | 5486 | C | HIS | 105 | 14.278 | 39.762 | 35.129 | 1.00 23.27 | CPS6 |
| ATOM | 5487 | 0 | HIS | 105 | 13.575 | 39.039 | 34.417 | 1.00 21.93 | CPS6 |
| ATOM | 5488 | N | THR | 106 | 13.837 | 40.393 | 36.212 | 1.00 23.40 | CPS6 |
| ATOM | 5489 | CA | THR | 106 | 12.430 | 40.421 | 36.605 | 1.00 25.56 | CPS6 |
| ATOM | 5490 | CB | THR | 106 | 12.067 | 39.537 | 37.816 | 1.00 27.06 | CPS6 |
| ATOM | 5491 | OGI | | 106 | 12.664 | 40.059 | 39.015 | 1.00 26.80 | CPS6 |
| ATOM | 5492 | CG2 | THR | 106 | 12.496 | 38.102 | 37.567 | 1.00 25.79 | CPS6 |
| ATOM | 5493 | C | THR | 106 | 12.266 | 41.879 | 37.013 | 1.00 27.51 | CPS6 |
| ATOM | 5494 | 0 | THR | 106 | 13.230 | 42.651 | 36.964 | 1.00 26.39 | CPS6 |
| ATOM | 5495 | N | LYS | 107 | 11.069 | 42.272 | 37.423 | 1.00 28.29 | CPS6 |
| ATOM | 5496 | CA | LYS | 107 | 10.880 | 43.662 | 37.810 | 1.00 29.88 | CPS6 |
| ATOM | 5497 | CB | LYS | 107 | 9.440 | 43.899 | 38.268 | 1.00 32.33 | CPS6 |
| ATOM | 5498 | CG | LYS | 107 | 9.155 | 45.357 | 38.599 | 1.00 36.25 | CPS6 |
| ATOM | 5499 | CD | LYS | 107 | 7.745 | 45.549 | 39.147 | 1.00 39.84 | CPS6 |
| ATOM | 5500 | CE | LYS | 107 | 7.473 | 47.024 | 39.442 | 1.00 41.42 | CPS6 |
| ATOM | 5501 | NZ | LYS | 107 | 6.102 | 47.246 | 39.995 | 1.00 45.05 | CPS6 |
| MOTA | 5502 | C | LYS | 107 | 11.839 | 44.132 | 38.905 | 1.00 29.50 | CPS6 |
| MOTA | 5503 | 0 | LYS | 107 | 12.367 | 45.243 | 38.823 | 1.00 29.28 | CPS6 |
| ATOM | 5504 | И | GLU | 108 | 12.081 | 43.289 | 39.912 | 1.00 27.21 | CPS6 |
| ATOM | 5505 | CA | GLU | 108 | 12.945 | 43.667 | 41.033 | 1.00 26.33 | CPS6 |
| | 5506 | CB | GLU | 108 | 12.239 | 43.363 | 42.358 | 1.00 30.27 | CPS6 |
| ATOM ATOM | 5507 | CG | GLU | 108 | 10.841 | 43.953 | 42.480 | 1.00 36.27 | CPS6 |
| ATOM | 5508 | CD | GLU | 108 | 10.259 | 43.782 | 43.874 | 1.00 41.02 | CPS6 |
| | 5509 | OE1 | | 108 | 10.158 | 42,632 | 44.354 | 1.00 44.74 | CPS6 |
| MOTA | 5510 | OE1 | | 108 | 9.897 | 44.803 | 44.497 | 1.00 45.09 | CPS6 |
| ATOM | | | GLU | 108 | 14.333 | 43.033 | 41.108 | 1.00 25.31 | CPS6 |
| ATOM | 5511 | C | GLU | 108 | 15.145 | 43.437 | 41.936 | 1.00 22.62 | CPS6 |
| ATOM | 5512 | 0 | TYR | 109 | 14.609 | 42.043 | 40.266 | 1.00 22.54 | CPS6 |
| ATOM | 5513 5514 | N | | | 15.900 | 41.368 | 40.333 | 1.00 22.99 | CPS6 |
| ATOM | | CA | TYR | 109 | 15.728 | 39.954 | 40.909 | 1.00 22.64 | CPS6 |
| MOTA | 5515 | CB | TYR | 109 | | 39.906 | 42.310 | 1.00 24.37 | CPS6 |
| MOTA | 5516 | CG | TYR | 109 | 15.175 15.988 | 40.167 | 43.411 | 1.00 24.51 | CPS6 |
| ATOM | 5517 | | TYR | 109 | | 40.190 | 44.701 | 1.00 26.40 | CPS6 |
| MOTA | 5518 | | TYR | 109 | 15.465 | | 42.531 | 1.00 24.67 | CPS6 |
| MOTA | 5519 | | TYR | 109 | 13.821 | 39.661 | 43.809 | 1.00 24.88 | CPS6 |
| ATOM | 5520 | CE2 | | 109 | 13.286 | 39.683 | | 1.00 24.88 | CPS6 |
| ATOM | 5521 | CZ | TYR | 109 | 14.106 | 39.946 | 44.884 | 1.00 29.07 | CPS6 |
| MOTA | 5522 | OH | TYR | 109 | 13.576 | 39.968 | 46.144 39.008 | 1.00 29.07 | CPS6 |
| ATOM | 5523 | C | TYR | 109 | 16.609 | 41.211 | | 1.00 21.70 | CPS6 |
| ATOM | 5524 | 0 | TYR | 109 | 15.993 | 41.280 | 37.945 | 1.00 22.34 | CPS6 |
| MOTA | 5525 | N | ALA | 110 | 17.926 | 41.012 | 39.103 | 1.00 20.16 | CPS6 |
| ATOM | 5526 | CA | ALA | 110 | 18.770 | 40.702 | 37.950 | 1.00 20.18 | CPS6 |
| ATOM | 5527 | CB | ALA | 110 | 19.785 | 41.803 | 37.666 | | CPS6 |
| MOTA | 5528 | C | ALA | 110 | 19.492 | 39.445 | 38.443 | 1.00 20.44 | CF30 |

| MOTA | 5529 | 0 | ALA | 110 | 19.824 | 39.345 | 39.621 | 1.00 21.38 | CPS6 |
|------|------|-----|-----|-----|--------|--------|--------|------------|--------------|
| MOTA | 5530 | N | ALA | 111 | 19.714 | 38.476 | 37.560 | 1.00 19.56 | CPS6 |
| MOTA | 5531 | CA | ALA | 111 | 20.415 | 37.272 | 37.962 | 1.00 17.92 | CPS6 |
| MOTA | 5532 | CB | ALA | 111 | 19.410 | 36.180 | 38.358 | 1.00 18.78 | CPS6 |
| ATOM | 5533 | C | ALA | 111 | 21.286 | 36.791 | 36.808 | 1.00 18.10 | CPS6 |
| ATOM | 5534 | 0 | ALA | 111 | 21.044 | 37.114 | 35.654 | 1.00 19.16 | CPS6 |
| MOTA | 5535 | N | ALA | 112 | 22.319 | 36.033 | 37.128 | 1.00 18.13 | CPS6 |
| ATOM | 5536 | CA | ALA | 112 | 23.175 | 35.509 | 36.083 | 1.00 18.42 | CPS6 |
| MOTA | 5537 | CB | ALA | 112 | 24.206 | 36.565 | 35.659 | 1.00 16.42 | CPS6 |
| MOTA | 5538 | С | ALA | 112 | 23.882 | 34.260 | 36.569 | 1.00 17.57 | CPS6 |
| MOTA | 5539 | 0 | ALA | 112 | 24.000 | 34.017 | 37.778 | 1.00 18.87 | CPS6 |
| ATOM | 5540 | N | GLN | 113 | 24.327 | 33.449 | 35.619 | 1.00 17.13 | CPS6 |
| ATOM | 5541 | CA | GLN | 113 | 25.065 | 32.247 | 35.971 | 1.00 17.77 | CPS6 |
| ATOM | 5542 | CB | GLN | 113 | 24.163 | 31.017 | 35.898 | 1.00 19.54 | CPS6 |
| ATOM | 5543 | CG | GLN | 113 | 23.699 | 30.693 | 34.495 | 1.00 21.95 | CPS6 |
| MOTA | 5544 | CD | GLN | 113 | 22.787 | 29.472 | 34.435 | 1.00 25.73 | CPS6 |
| MOTA | 5545 | OEl | GLN | 113 | 22.446 | 29.002 | 33.352 | 1.00 27.72 | CPS6 |
| MOTA | 5546 | NE2 | GLN | 113 | 22.378 | 28.968 | 35.594 | 1.00 27.67 | CPS6 |
| MOTA | 5547 | С | GLN | 113 | 26.205 | 32.133 | 34.968 | 1.00 16.69 | CPS6 |
| ATOM | 5548 | 0 | GLN | 113 | 26.104 | 32.622 | 33.840 | 1.00 16.20 | CPS6 |
| ATOM | 5549 | N | VAL | 114 | 27.288 | 31.499 | 35.391 | 1.00 17.22 | CPS6 |
| ATOM | 5550 | CA | VAL | 114 | 28.449 | 31.324 | 34.535 | 1.00 17.47 | CPS6 |
| ATOM | 5551 | CB | VAL | 114 | 29.605 | 32.300 | 34.948 | 1.00 17.72 | CPS6 |
| ATOM | 5552 | CG1 | VAL | 114 | 30.931 | 31.901 | 34.243 | 1.00 16.56 | CPS6 |
| ATOM | 5553 | CG2 | VAL | 114 | 29.222 | 33.738 | 34.581 | 1.00 17.27 | CPS6 |
| ATOM | 5554 | C | VAL | 114 | 28.964 | 29.911 | 34.693 | 1.00 18.72 | CPS6 |
| ATOM | 5555 | 0 | VAL | 114 | 28.880 | 29.338 | 35.776 | 1.00 19.21 | CPS6 |
| ATOM | 5556 | N | VAL | 115 | 29.461 | 29.338 | 33.604 | 1.00 18.94 | CPS6 |
| MOTA | 5557 | CA | VAL | 115 | 30.090 | 28.027 | 33.684 | 1.00 19.93 | CPS6 |
| MOTA | 5558 | CB | VAL | 115 | 29.311 | 26.916 | 32.928 | 1.00 19.40 | CPS6 |
| MOTA | 5559 | CG1 | VAL | 115 | 30.143 | 25.631 | 32.901 | 1.00 20.42 | CPS6 |
| MOTA | 5560 | CG2 | LAV | 115 | 27.981 | 26.638 | 33.628 | 1.00 19.61 | CPS6 |
| MOTA | 5561 | C | LAV | 115 | 31.453 | 28.231 | 33.023 | 1.00 20.14 | CPS6 |
| ATOM | 5562 | 0 | VAL | 115 | 31.562 | 28.860 | 31.958 | 1.00 19.69 | CPS6 |
| MOTA | 5563 | N | ILE | 116 | 32.498 | 27.750 | 33.680 | 1.00 19.47 | CPS6 |
| ATOM | 5564 | CA | ILE | 116 | 33.839 | 27.853 | 33.121 | 1.00 21.42 | CPS6 |
| ATOM | 5565 | CB | ILE | 116 | 34.806 | 28.617 | 34.068 | 1.00 21.08 | CPS6 |
| ATOM | 5566 | CG2 | ILE | 116 | 36.235 | 28.577 | 33.505 | 1.00 23.06 | CPS6 |
| MOTA | 5567 | CG1 | ILE | 116 | 34.365 | 30.082 | 34.195 | 1.00 21.71 | CPS6 |
| ATOM | 5568 | CD1 | ILE | 116 | 35.180 | 30.906 | 35.213 | 1.00 21.07 | CPS6 |
| ATOM | 5569 | C | ILE | 116 | 34.320 | 26.420 | 32.940 | 1.00 24.10 | CPS6 |
| ATOM | 5570 | 0 | ILE | 116 | 34.264 | 25.615 | 33.872 | 1.00 23.26 | CPS6 |
| ATOM | 5571 | N | GLU | 117 | 34.759 | 26.103 | 31.731 | 1.00 25.26 | CPS6 |
| MOTA | 5572 | CA | GLU | 117 | 35.243 | 24.769 | 31.424 | 1.00 29.11 | CPS6 |
| MOTA | 5573 | CB | GLU | 117 | 34.878 | 24.369 | 30.001 | 1.00 30.47 | CPS6 |
| MOTA | 5574 | CG | GLU | 117 | 33.446 | 24.548 | 29.587 | 1.00 33.45 | CPS6 |
| ATOM | 5575 | CD | GLU | 117 | 33.226 | 24.007 | 28.194 | 1.00 36.82 | CPS6 |
| ATOM | 5576 | | GLU | 117 | 33.345 | 22.776 | 28.022 | 1.00 39.37 | CPS6 |
| ATOM | 5577 | | GLU | 117 | 32.959 | 24.804 | 27.271 | 1.00 38.14 | CPS6 |
| ATOM | 5578 | C | GLU | 117 | 36.754 | 24.698 | 31.503 | 1.00 31.19 | CPS6 |
| ATOM | 5579 | 0 | GLU | 117 | 37.445 | 25.712 | 31.392 | 1.00 28.72 | CPS6 |
| ATOM | 5580 | N | ARG | 118 | 37.259 | 23.484 | 31.686 | 1.00 34.06 | CPS6 |
| ATOM | 5581 | CA | ARG | 118 | 38.692 | 23.267 | 31.686 | 1.00 39.18 | CPS6 |
| ATOM | 5582 | CB | ARG | 118 | 39.089 | 22.180 | 32.703 | 1.00 40.91 | CPS6 |
| ATOM | 5583 | CG | ARG | 118 | 38.327 | 20.872 | 32.574 | 1.00 46.37 | CPS6 CPS6 |
| MOTA | 5584 | CD | ARG | 118 | 38.840 | 19.776 | 33.528 | 1.00 49.12 | CPS6 |
| MOTA | 5585 | NE | ARG | 118 | 38.479 | 19.996 | 34.930 | 1.00 50.78 | CPS6 |

| ATOM | 5586 | CZ | ARG | 118 | 39.095 | 20.849 | 35.744 | 1.00 51.80 | CPS6 |
|------|--------------|-----|-----|-----|--------|--------|---------|------------|----------|
| ATOM | 5587 | NHl | | 118 | 40.113 | 21.575 | 35.304 | 1.00 53.03 | CPS6 |
| MOTA | 5588 | NH2 | ARG | 118 | 38.692 | 20.977 | 37.003 | 1.00 51.56 | CPS6 |
| MOTA | 5589 | C | ARG | 118 | 38.895 | 22.789 | 30.250 | 1.00 40.50 | CPS6 |
| ATOM | 5590 | 0 | ARG | 118 | 38.365 | 21.750 | 29.862 | 1.00 41.56 | CPS6 |
| ATOM | 5591 | N | LEU | 119 | 39.615 | 23.562 | 29.445 | 1.00 42.65 | CPS6 |
| ATOM | 5592 | CA | LEU | 119 | 39.833 | 23.176 | 28.055 | 1.00 44.91 | CPS6 |
| ATOM | 5593 | CB | LEU | 119 | 40.106 | 24.414 | 27.196 | 1.00 45.15 | CPS6 |
| ATOM | 5594 | CG | LEU | 119 | 38.970 | 25.432 | 27.070 | 1.00 45.37 | CPS6 |
| MOTA | 5595 | | LEU | 119 | 39.442 | 26.618 | 26.246 | 1.00 44.17 | CPS6 |
| ATOM | 5596 | | LEU | 119 | 37.752 | 24.776 | 26.427 | 1.00 45.02 | CPS6 |
| ATOM | 5597 | C | LEU | 119 | 40.991 | 22.193 | 27.918 | 1.00 45.02 | CPS6 |
| | | | | | 41.823 | | | 1.00 45.41 | |
| ATOM | 5598 | | LEU | 119 | | 22.138 | 28.848 | | CPS6 |
| ATOM | 5599 | | LEU | 119 | 41.055 | 21.501 | 26.874 | 1.00 47.76 | CPS6 |
| ATOM | 5600 | 0 | НОН | 1 | 74.183 | | -19.320 | 1.00 16.24 | AT |
| MOTA | 5601 | 0 | нон | 2 | 50.451 | 28.498 | 2.245 | 1.00 16.26 | AT |
| MOTA | 5602 | 0 | HOH | 3 | 72.513 | 43.845 | 5.247 | 1.00 16.95 | AT |
| MOTA | 5603 | 0 | HOH | 4 | 59.768 | 49.591 | 13.381 | 1.00 18.99 | AT |
| ATOM | 5604 | 0 | HOH | 5 | 9.919 | 40.963 | 40.359 | 1.00 17.22 | AT |
| MOTA | 5605 | 0 | HOH | 6 | 57.301 | 49.721 | 15.536 | 1.00 18.51 | TA |
| MOTA | 560 6 | 0 | HOH | 7 | 72.254 | 36.424 | 22.184 | 1.00 19.44 | AT |
| MOTA | 5607 | 0 | HOH | . 8 | 15.486 | 40.288 | 48.189 | 1.00 19.00 | AT |
| MOTA | 5608 | 0 | HOH | 9 | 22.359 | 26.422 | 33.132 | 1.00 28.69 | AT |
| ATOM | 5609 | 0 | HOH | 10 | 62.648 | 41.000 | 12.765 | 1.00 26.69 | AT |
| ATOM | 5610 | 0 | HOH | 11 | 27.253 | 11.532 | 60.836 | 1.00 33.03 | AT |
| ATOM | 5611 | 0 | нон | 12 | 4.545 | 29.482 | 16.753 | 1.00 34.49 | TA |
| ATOM | 5612 | 0 | нон | 13 | 14.678 | 33.346 | 17.568 | 1.00 28.16 | AT |
| ATOM | 5613 | 0 | нон | 14 | 2.443 | 17.966 | 21.642 | 1.00 31.50 | AT |
| MOTA | 5614 | 0 | HOH | 15 | 13.387 | 44.897 | 46.109 | 1.00 36.84 | ΑT |
| ATOM | 5615 | ō | нон | 16 | 64.048 | 43.971 | 9.189 | 1.00 27.36 | AT |
| ATOM | 5616 | o | нон | 17 | 17.153 | 29.081 | 61.693 | 1.00 38.80 | AT |
| ATOM | 5617 | 0 | нон | 18 | 15.565 | 11.097 | 37.041 | 1.00 32.04 | TA |
| | | | HOH | 19 | 66.736 | 39.802 | 9.758 | 1.00 32.04 | AT |
| ATOM | 5618 | 0 | | | | 35.163 | 19.609 | 1.00 43.12 | AT |
| ATOM | 5619 | 0 | HOH | 20 | 68.806 | | | | AT |
| MOTA | 5620 | 0 | HOH | 21 | 28.442 | 30.448 | 25.270 | 1.00 35.30 | |
| ATOM | 5621 | 0 | HOH | 22 | 20.356 | 37.769 | 28.103 | 1.00 40.41 | AT |
| ATOM | 5622 | 0 | HOH | 23 | 27.784 | 56.284 | 42.007 | 1.00 39.44 | AT |
| ATOM | 5623 | 0 | HOH | 24 | 9.819 | 21.853 | 51.711 | 1.00 48.93 | AT |
| ATOM | 5624 | 0 | нон | 25 | 18.794 | 48.571 | 49.608 | 1.00 38.44 | AT |
| MOTA | 5625 | 0 | HOH | 26 | 50.953 | 43.970 | 28.198 | 1.00 29.58 | AT |
| MOTA | 5626 | 0 | HOH | 27 | 22.120 | 28.021 | 18.001 | 1.00 41.70 | AT |
| MOTA | 5627 | 0 | HOH | 28 | 18.224 | 7.825 | 50.971 | 1.00 37.65 | AT |
| ATOM | 5628 | 0 | HOH | 29 | 45.010 | 40.785 | 1.909 | 1.00 35.18 | AT |
| MOTA | 5629 | 0 | HOH | 30 | 64.211 | 31.229 | 23.988 | 1.00 42.82 | TA |
| MOTA | 5630 | 0 | HOH | 31 | 55.673 | 59.846 | 2.934 | 1.00 40.75 | AT |
| MOTA | 5631 | 0 | нон | 32 | 12.144 | 16.656 | 71.990 | 1.00 45.41 | AT |
| MOTA | 5632 | 0 | HOH | 33 | 26.174 | 28.070 | 35.889 | 1.00 33.23 | AT |
| ATOM | 5633 | 0 | нон | 34 | 23.423 | 24.108 | 37.385 | 1.00 33.85 | AT |
| ATOM | 5634 | 0 | нон | 35 | 72.206 | 58.375 | 9.452 | 1.00 45.41 | AT |
| ATOM | 5635 | Ö | НОН | 36 | 4.583 | 28.820 | 43.211 | 1.00 37.91 | TA |
| ATOM | 5636 | 0 | нон | 37 | 54.428 | 31.469 | 26.691 | 1.00 40.61 | AT |
| ATOM | 5637 | 0 | НОН | 38 | 5.129 | 39.360 | 42.159 | 1.00 34.31 | AT |
| | 5638 | 0 | HOH | 39 | 61.288 | 9.543 | 3.422 | 1.00 45.78 | AT |
| ATOM | | | | | | | | 1.00 46.77 | AT |
| ATOM | 5639 | 0 | HOH | 40 | 41.144 | 21.554 | 50.056 | 1.00 46.77 | AT |
| ATOM | 5640 | 0 | нон | 41 | 45.899 | 31.375 | 23.218 | 1.00 40.88 | AT TA |
| ATOM | 5641 | 0 | нон | 42 | 46.684 | 40.019 | 4.072 | | |
| ATOM | 5642 | 0 | HOH | 43 | 32.060 | 30.436 | 24.972 | 1.00 38.00 | AT |

| ATOM | 5643 | 0 | нон | 44 | 27.193 | 55.260 | 39.276 | 1.00 39.83 | AT |
|--------|------|---|-----|-----|--------|--------|--------|------------|----------|
| ATOM | 5644 | Ō | нон | 45 | 74.083 | 12.016 | 10.419 | 1.00 37.57 | AT |
| ATOM | 5645 | ō | нон | 46 | 7.161 | 11.806 | 20.918 | 1.00 37.37 | AT AT |
| ATOM | 5646 | ŏ | нон | 47 | 37.597 | 37.224 | 10.717 | 1.00 37.74 | |
| ATOM | 5647 | Ö | нон | 48 | 26.713 | 40.428 | 46.123 | | AT |
| ATOM | 5648 | 0 | нон | 49 | 73.327 | 31.524 | 18.039 | 1.00 47.01 | AT |
| | | 0 | | 50 | | | | 1.00 39.95 | AT |
| ATOM | 5649 | | HOH | | 6.885 | 35.701 | 48.910 | 1.00 38.11 | AT |
| ATOM | 5650 | 0 | HOH | 51 | 12.147 | 30.555 | 62.867 | 1.00 45.67 | AT |
| ATOM | 5651 | 0 | нон | 52 | 45.035 | 35.126 | 28.209 | 1.00 45.09 | AT |
| ATOM | 5652 | 0 | нон | 53 | 45.816 | 30.463 | 0.531 | 1.00 37.06 | AT |
| ATOM | 5653 | 0 | нон | 54 | 37.959 | 49.546 | 12.787 | 1.00 41.97 | AT |
| MOTA | 5654 | 0 | HOH | 55 | 29.307 | 59.252 | 40.586 | 1.00 54.29 | AT |
| MOTA | 5655 | 0 | HOH | 56 | 33.064 | 30.245 | 14.482 | 1.00 53.18 | TA |
| MOTA | 5656 | 0 | нон | 57 | 5.959 | 29.404 | 40.923 | 1.00 42.88 | AT |
| MOTA | 5657 | 0 | нон | 58 | 72.015 | 56.594 | 2.111 | 1.00 41.98 | AT |
| MOTA | 5658 | 0 | HOH | 59 | 34.149 | 9.199 | 46.267 | 1.00 42.25 | AT |
| MOTA | 5659 | 0 | HOH | 60 | 56.871 | 24.901 | 5.890 | 1.00 43.48 | TA |
| MOTA | 5660 | 0 | HOH | 61 | 53.366 | 27.278 | 27.533 | 1.00 46.43 | AT |
| ATOM | 5661 | 0 | HOH | 62 | 51.684 | 37.046 | 30.830 | 1.00 46.25 | AT |
| ATOM | 5662 | 0 | HOH | 63 | 52.569 | 48.531 | 8.124 | 1.00 42.45 | AT |
| ATOM | 5663 | 0 | HOH | 64 | 19.990 | 15.518 | 32.236 | 1.00 48.76 | AT |
| MOTA | 5664 | 0 | HOH | 65 | 64.540 | 44.979 | 26.386 | 1.00 42.49 | AT |
| MOTA | 5665 | 0 | HOH | 66 | 30.220 | 13.054 | 46.228 | 1.00 52.13 | AT |
| ATOM | 5666 | 0 | HOH | 67 | 54.239 | 52.985 | 1.438 | 1.00 45.12 | ΤA |
| ATOM | 5667 | 0 | HOH | 68 | 20.023 | 54.748 | 37.127 | 1.00 39.76 | TA |
| ATOM | 5668 | 0 | HOH | 69 | 8.456 | 21.336 | 37.515 | 1.00 48.76 | TA |
| MOTA | 5669 | 0 | HOH | 70 | 35.909 | 45.522 | 2.599 | 1.00 46.39 | TA |
| MOTA | 5670 | 0 | HOH | 71 | 53.886 | 30.997 | 19.731 | 1.00 43.92 | AT |
| MOTA | 5671 | 0 | HOH | 72 | 10.033 | 24.488 | 66.210 | 1.00 53.66 | ΑT |
| MOTA | 5672 | 0 | HOH | 73 | 58.903 | 57.250 | 13.037 | 1.00 41.23 | AT |
| MOTA | 5673 | 0 | HOH | 74 | 62.777 | 15.875 | 1.984 | 1.00 41.20 | AT |
| ATOM | 5674 | 0 | HOH | 75 | 42.217 | 40.323 | 33.742 | 1.00 43.11 | AT |
| MOTA | 5675 | 0 | HOH | 76 | 20.956 | 40.692 | 29.179 | 1.00 49.81 | AT |
| ATOM | 5676 | 0 | HOH | 77 | 46.166 | 43.977 | 11.730 | 1.00 36.26 | AT |
| ATOM | 5677 | 0 | HOH | 78 | 66.744 | 59.058 | 16.145 | 1.00 56.18 | AT |
| ATOM | 5678 | 0 | HOH | 79 | 45.851 | 25.881 | 4.391 | 1.00 55.88 | TA |
| ATOM | 5679 | 0 | HOH | 80 | 75.174 | 49.183 | 6.063 | 1.00 47.74 | TA |
| ATOM | 5680 | 0 | HOH | 81 | 29.310 | 41.802 | 17.220 | 1.00 55.92 | AT |
| ATOM | 5681 | 0 | HOH | 82 | 1.927 | 35.649 | 42.778 | 1.00 51.25 | AT |
| ATOM | 5682 | 0 | HOH | 83 | -1.663 | 38.805 | 38.155 | 1.00 39.95 | AT |
| MOTA | 5683 | 0 | HOH | 84 | 14.052 | 11.606 | 52.410 | 1.00 45.64 | AT |
| MOTA | 5684 | 0 | HOH | 85 | 12.374 | 37.222 | 15.756 | 1.00 49.24 | AT |
| MOTA | 5685 | 0 | HOH | 86 | 31.903 | 41.930 | 45.468 | 1.00 45.19 | AT |
| ATOM | 5686 | 0 | HOH | 87 | 33.483 | 20.380 | 56.292 | 1.00 53.83 | AT |
| ATOM | 5687 | 0 | HOH | 88 | 74.639 | 45.461 | 5.020 | 1.00 41.59 | AT |
| ATOM | 5688 | 0 | HOH | 89 | 37.028 | 19.108 | 53.278 | 1.00 43.77 | AT |
| ATOM | 5689 | 0 | нон | 90 | 38.593 | 49.011 | 6.342 | 1.00 51.49 | AT |
| ATOM | 5690 | 0 | HOH | 91 | 52.402 | 56.617 | 3.593 | 1.00 53.57 | TA |
| ATOM | 5691 | 0 | нон | 92 | 5.772 | 28.675 | 61.930 | 1.00 44.14 | TA |
| ATOM | 5692 | 0 | нон | 93 | 32.173 | 36.302 | 19.628 | 1.00 45.70 | AT |
| ATOM | 5693 | 0 | HOH | 94 | 52.026 | 42.123 | 29.953 | 1.00 47.73 | TA |
| ATOM | 5694 | ō | НОН | 95 | 47.042 | 40.027 | 29.849 | 1.00 57.66 | AT |
| ATOM | 5695 | Ö | нон | 96 | 62.041 | 43.614 | 30.370 | 1.00 49.31 | AT |
| ATOM | 5696 | ō | нон | 97 | 61.630 | 30.997 | 18.476 | 1.00 53.79 | AT |
| ATOM | 5697 | Ö | нон | 98 | 11.168 | 13.661 | 45.409 | 1.00 45.46 | AT |
| MOTA | 5698 | Ö | нон | 99 | 28.738 | 15.678 | 20.064 | 1.00 63.95 | AT |
| ATOM | 5699 | Ö | нон | 100 | 37.162 | 57.858 | 42.839 | 1.00 49.29 | AT |
| 212011 | 2222 | ~ | | | 57.202 | 37.030 | | · - · · | |

| MOTA | 5700 | 0 | HOH | 101 | 56.970 | 48.398 | 18.183 | 1.00 20.07 | AT |
|------|------|---|-----|-----|--------|------------------|------------------|--------------------------|------------------------|
| MOTA | 5701 | 0 | HOH | 102 | 16.747 | 17.196 | 32.059 | 1.00 21.58 | AT |
| ATOM | 5702 | 0 | HOH | 103 | 45.835 | 52.603 | 17.631 | 1.00 19.92 | AT |
| ATOM | 5703 | 0 | HOH | 104 | -5.526 | 20.298 | 17.919 | 1.00 20.40 | AT |
| ATOM | 5704 | 0 | HOH | 105 | 16.573 | 18.225 | 29.320 | 1.00 21.11 | AT |
| ATOM | 5705 | 0 | HOH | 106 | 28.084 | 33.122 | 26.572 | 1.00 21.96 | AΤ |
| MOTA | 5706 | 0 | HOH | 107 | 56.776 | 49.897 | 20.691 | 1.00 20.77 | AT |
| ATOM | 5707 | 0 | HOH | 108 | 61.822 | 31.586 | 15.608 | 1.00 22.44 | AT |
| MOTA | 5708 | 0 | HOH | 109 | 75.499 | 25.254 | 21.262 | 1.00 22.49 | AT |
| ATOM | 5709 | 0 | HOH | 110 | 52.716 | 36.178 | -8.615 | 1.00 23.96 | AT |
| ATOM | 5710 | 0 | HOH | 111 | 30.657 | 33.717 | 27.675 | 1.00 22.13 | AT |
| MOTA | 5711 | 0 | HOH | 112 | 31.857 | 23.322 | 43.883 | 1.00 22.91 | AT |
| MOTA | 5712 | 0 | HOH | 113 | 16.560 | 16.176 | 27.250 | 1.00 22.50 | AΤ |
| ATOM | 5713 | 0 | нон | 114 | 48.919 | 55.521 | 18.754 | 1.00 22.71 | AT |
| MOTA | 5714 | 0 | нон | 115 | 30.469 | 45.806 | 26.160 | 1.00 24.06 | AT |
| MOTA | 5715 | 0 | нон | 116 | 29.611 | 29.912 | 44.889 | 1.00 23.26 | AT |
| MOTA | 5716 | 0 | HOH | 117 | 14.658 | 45.605 | 43.596 | 1.00 25.77 | AT |
| ATOM | 5717 | 0 | HOH | 118 | 38.482 | 35.704 | 27.602 | 1.00 23.84 | AT |
| ATOM | 5718 | 0 | HOH | 119 | 33.048 | 33.856 | 26.010 | 1.00 23.17 | $\mathbf{T}\mathbf{A}$ |
| ATOM | 5719 | 0 | HOH | 120 | 11.956 | 35.757 | 52.609 | 1.00 26.32 | AT |
| MOTA | 5720 | 0 | HOH | 121 | 72.585 | 45.998 | 2.976 | 1.00 23.39 | AT |
| MOTA | 5721 | 0 | HOH | 122 | 45.040 | 32.707 | 1.982 | 1.00 25.55 | AT |
| ATOM | 5722 | 0 | HOH | 123 | 71.609 | 48.727 | 2.944 | 1.00 24.67 | AT |
| ATOM | 5723 | 0 | HOH | 124 | 34.369 | 7.558 | 43.913 | 1.00 24.87 | AT |
| ATOM | 5724 | 0 | HOH | 125 | 4.595 | 36.818 | 41.429 | 1.00 25.98 | TA |
| MOTA | 5725 | 0 | HOH | 126 | 11.206 | 23.871 | 43.608 | 1.00 25.23 | AT |
| MOTA | 5726 | 0 | HOH | 127 | 14.284 | 14.636 | 65.129 | 1.00 25.02 | AT |
| MOTA | 5727 | 0 | HOH | 128 | 70.983 | 32.077 | 16.439 | 1.00 25.53 | $\mathtt{T}\mathtt{A}$ |
| ATOM | 5728 | 0 | HOH | 129 | 15.935 | 10.066 | 59.658 | 1.00 25.84 | ΑT |
| MOTA | 5729 | 0 | HOH | 130 | 17.042 | 11.420 | 57.203 | 1.00 25.22 | AΤ |
| MOTA | 5730 | 0 | HOH | 131 | 78.508 | 30.572 | 16.070 | 1.00 25.80 | AT |
| MOTA | 5731 | 0 | HOH | 132 | 31.882 | 25.438 | 41.276 | 1.00 25.44 | AT |
| MOTA | 5732 | 0 | HOH | 133 | 68.333 | 21.576 | 13.174 | 1.00 27.25 | AT |
| MOTA | 5733 | 0 | HOH | 134 | 59.808 | 51.543 | 15.137 | 1.00 26.71 | AT |
| ATOM | 5734 | 0 | HOH | 135 | 51.803 | 45.823 | 2.829 | 1.00 28.23 | AT |
| MOTA | 5735 | 0 | HOH | 136 | 23.948 | 33.437 | 19.543 | 1.00 26.93 | TA |
| MOTA | 5736 | 0 | HOH | 137 | 77.529 | 24.686 | -0.187 | 1.00 27.06 | AT |
| MOTA | 5737 | 0 | HOH | 138 | 36.414 | 47.961 | 27.068 | 1.00 26.59 | AT |
| MOTA | 5738 | 0 | HOH | 139 | 15.210 | 37.727 | 30.916 | 1.00 26.63 | AT |
| MOTA | 5739 | 0 | нон | 140 | 26.736 | 13.803 | 59.642 | 1.00 27.51 | TA |
| ATOM | 5740 | 0 | HOH | 141 | 59.707 | 29.029 | -5.923 | 1.00 28.00 | AT |
| ATOM | 5741 | 0 | HOH | 142 | 73.385 | 50.907 | 2.916 | 1.00 25.70 | AT |
| ATOM | 5742 | 0 | нон | 143 | 25.372 | 31.413 | 54.764 | 1.00 28.23 | AT |
| MOTA | 5743 | 0 | нон | 144 | 8.726 | 40.753 | 36.473 | 1.00 28.04 | AT |
| MOTA | 5744 | 0 | HOH | 145 | 21.631 | 52.226 | 39.835 | 1.00 27.68 | AT AT |
| MOTA | 5745 | 0 | HOH | 146 | 6.966 | 31.512 | 19.584 | 1.00 26.22 | AT |
| MOTA | 5746 | 0 | нон | 147 | 33.568 | 23.343 | 41.390 | 1.00 28.59 | AT AT |
| ATOM | 5747 | 0 | нон | 148 | 47.104 | 33.497 | 24,474 | 1.00 31.57 | |
| ATOM | 5748 | 0 | HOH | 149 | 42.706 | 46.788 | 25.123 53.744 | 1.00 28.27 1.00 28.43 | AT AT |
| ATOM | 5749 | 0 | HOH | 150 | 15.361 | 13.776 | | 1.00 26.48 | AT |
| MOTA | 5750 | 0 | HOH | 151 | 49.210 | 27.704 37.893 | 6.023 23.208 | 1.00 28.48 | AT |
| MOTA | 5751 | 0 | HOH | 152 | 69.742 | | 28.207 | 1.00 28.03 | AT |
| MOTA | 5752 | 0 | HOH | 153 | 62.896 | 46.941 | -2.754 | 1.00 27.04 | AT |
| ATOM | 5753 | 0 | HOH | 154 | 66.194 | 34.304 | 12.351 | 1.00 27.04 | AT |
| ATOM | 5754 | 0 | HOH | 155 | 56.380 | 56.783 | 9.697 | 1.00 29.49 | AT |
| ATOM | 5755 | 0 | HOH | 156 | 62.810 | 23.721 | -20.735 | 1.00 30.39 | AT |
| ATOM | 5756 | 0 | нон | 157 | 59.600 | 40.020 | -20.133 | 1.00 30.33 | |

| MOTA | 5757 | 0 | HOH | 158 | 63.447 | 33.873 | 17.572 | 1.00 29.71 | AT |
|------|------|---|-----|-----|--------|--------|---------|------------|---------------|
| MOTA | 5758 | 0 | HOH | 159 | 11.724 | 13.599 | 66.211 | 1.00 27.82 | AT |
| ATOM | 5759 | 0 | нон | 160 | 60.558 | 22.006 | 10.718 | 1.00 28.85 | AT |
| ATOM | 5760 | 0 | нон | 161 | 46.499 | 54.700 | 19.899 | 1.00 29.19 | AT |
| ATOM | 5761 | o | нон | 162 | 63.410 | 57.441 | | 1.00 29.14 | AT |
| ATOM | 5762 | 0 | нон | 163 | 16.531 | 13.383 | 27.915 | 1.00 29.14 | |
| | | | | | 57.094 | | | | TA |
| ATOM | 5763 | 0 | нон | 164 | | 58.123 | -5.057 | 1.00 30.67 | AT |
| MOTA | 5764 | 0 | HOH | 165 | 55.029 | 24.601 | -1.884 | 1.00 27.07 | AT |
| MOTA | 5765 | 0 | HOH | 166 | 13.338 | 35.151 | 24.133 | 1.00 28.54 | AT |
| ATOM | 5766 | 0 | HOH | 167 | 35.398 | 47.783 | 6.493 | 1.00 28.26 | TA |
| ATOM | 5767 | 0 | HOH | 168 | 70.174 | 56.885 | -10.515 | 1.00 31.78 | AT |
| ATOM | 5768 | 0 | HOH | 169 | 25.901 | 44.946 | 25.667 | 1.00 31.94 | AT |
| ATOM | 5769 | 0 | HOH | 170 | 50.393 | 53.846 | 23.119 | 1.00 28.26 | AT |
| ATOM | 5770 | 0 | HOH | 171 | 62.156 | 25.716 | 13.450 | 1.00 31.00 | AT |
| MOTA | 5771 | 0 | HOH | 172 | 42.474 | 44.185 | 26.823 | 1.00 31.95 | AT |
| ATOM | 5772 | 0 | нон | 173 | 77.820 | 49.020 | -5.810 | 1.00 32.32 | AT |
| ATOM | 5773 | Ö | нон | 174 | 67.420 | 39.148 | | 1.00 29.68 | AT |
| ATOM | 5774 | 0 | нон | 175 | 48.791 | 40.644 | -3.702 | 1.00 28.90 | TA |
| ATOM | 5775 | 0 | нон | 176 | 33.117 | 16.234 | 43.002 | 1.00 28.30 | AT |
| | | | | | | | | | |
| ATOM | 5776 | 0 | нон | 177 | 15.122 | 24.092 | 63.819 | 1.00 30.47 | AT |
| MOTA | 5777 | 0 | нон | 178 | 64.991 | 30.299 | -1.464 | 1.00 30.76 | AT |
| MOTA | 5778 | 0 | HOH | 179 | 15.212 | 16.862 | 21.098 | 1.00 32.61 | AT |
| ATOM | 5779 | 0 | HOH | 180 | 8.026 | 30.440 | 48.746 | 1.00 29.36 | AT |
| ATOM | 5780 | 0 | HOH | 181 | 15.063 | 29.611 | 60.193 | 1.00 29.52 | TA |
| MOTA | 5781 | 0 | HOH | 182 | -4.236 | 31.973 | 27.775 | 1.00 33.07 | AT |
| MOTA | 5782 | 0 | HOH | 183 | 41.379 | 28.581 | 29.607 | 1.00 31.08 | \mathtt{AT} |
| MOTA | 5783 | 0 | HOH | 184 | 30.685 | 20.525 | 44.633 | 1.00 30.33 | AT |
| MOTA | 5784 | 0 | HOH | 185 | 25.786 | 35.845 | 47.678 | 1.00 31.51 | AT |
| ATOM | 5785 | 0 | HOH | 186 | 33.235 | 47.941 | 17.895 | 1.00 29.68 | AT |
| ATOM | 5786 | 0 | HOH | 187 | 64.882 | 30.921 | 17.515 | 1.00 30.10 | AT |
| ATOM | 5787 | 0 | НОН | 188 | 5.685 | 13.963 | 30.264 | 1.00 32.30 | AT |
| ATOM | 5788 | 0 | нон | 189 | -4.735 | 20.413 | 39.978 | 1.00 33.19 | AT |
| MOTA | 5789 | ō | нон | 190 | 44.587 | 45.272 | 8.578 | 1.00 31.21 | AT |
| ATOM | 5790 | ō | НОН | 191 | 57.838 | 12.743 | 11.965 | 1.00 31.57 | AT |
| ATOM | 5791 | Õ | нон | 192 | 16.393 | 22.844 | 66.100 | 1.00 34.23 | AT |
| ATOM | 5792 | Ö | нон | 193 | 4.372 | 22.943 | 37.792 | 1.00 32.96 | TA |
| ATOM | 5793 | 0 | нон | 194 | 71.929 | 20.305 | 14.473 | 1.00 32.09 | AT |
| | | | | | | | 59.281 | 1.00 32.03 | AT |
| ATOM | 5794 | 0 | нон | 195 | 28.925 | 15.553 | | | AT |
| MOTA | 5795 | 0 | нон | 196 | 53.796 | 25.895 | -4.052 | 1.00 33.01 | |
| MOTA | 5796 | 0 | нон | 197 | 6.468 | 23.780 | 36.296 | 1.00 34.02 | AT |
| MOTA | 5797 | 0 | HOH | 198 | 53.710 | 44.972 | -1.506 | 1.00 33.84 | TA |
| MOTA | 5798 | 0 | HOH | 199 | 19.319 | 42.034 | 48.498 | 1.00 31.81 | TA |
| MOTA | 5799 | 0 | HOH | 200 | 24.603 | 12.893 | 57.779 | 1.00 32.45 | AT |
| ATOM | 5800 | 0 | нон | 201 | 82.186 | 45.693 | -2.681 | 1.00 34.17 | AT |
| MOTA | 5801 | 0 | HOH | 202 | 11.264 | 18.716 | 60.799 | 1.00 36.53 | AT |
| MOTA | 5802 | 0 | HOH | 203 | 79.085 | 17.668 | 9.255 | 1.00 31.67 | AT |
| ATOM | 5803 | 0 | HOH | 204 | 59.866 | 52.931 | 11.834 | 1.00 30.91 | AT |
| ATOM | 5804 | 0 | HOH | 205 | 13.907 | 16.278 | 62.855 | 1.00 36.18 | TA |
| MOTA | 5805 | 0 | HOH | 206 | 16.412 | 14.129 | 56.660 | 1.00 32.42 | AT |
| ATOM | 5806 | 0 | нон | 207 | 66.234 | 40.890 | -9.847 | 1.00 31.86 | AT |
| ATOM | 5807 | ō | нон | 208 | 10.481 | 11.237 | 25.068 | 1.00 32.03 | AT |
| MOTA | 5808 | 0 | нон | 209 | 5.289 | 19.707 | 30.585 | 1.00 33.17 | AT |
| ATOM | 5809 | 0 | нон | 210 | 39.446 | 40.017 | 23.668 | 1.00 33.18 | AT |
| | | | | | | | 6.035 | 1.00 35.31 | AT |
| ATOM | 5810 | 0 | HOH | 211 | 54.509 | 23.461 | | 1.00 33.31 | AT |
| ATOM | 5811 | 0 | HOH | 212 | 51.401 | 31.567 | 11.354 | 1.00 32.73 | AT |
| ATOM | 5812 | 0 | нон | 213 | 28.205 | 23.736 | 55.152 | | |
| ATOM | 5813 | 0 | HOH | 214 | 50.324 | 34.946 | -7.659 | 1.00 34.98 | TA |

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| ATOM | 5814 | 0 | нон | 215 | 30.129 | 20.719 | 56.661 | 1.00 32.37 | AT |
|------|------|---|-----|------------|--------|------------------|------------------|--------------------------|----------|
| MOTA | 5815 | 0 | HOH | 216 | 58.457 | 50.516 | -18.849 | 1.00 32.27 | AT |
| MOTA | 5816 | 0 | HOH | 217 | 44.476 | 34.908 | 24.562 | 1.00 35.00 | AT |
| MOTA | 5817 | 0 | HOH | 218 | 9.990 | 35.693 | 24.724 | 1.00 34.96 | TA |
| MOTA | 5818 | 0 | HOH | 219 | 11.096 | 35.811 | 32.093 | 1.00 34.27 | AT |
| MOTA | 5819 | 0 | HOH | 220 | 12.913 | 17.730 | 46.309 | 1.00 34.71 | AT |
| MOTA | 5820 | 0 | HOH | 221 | 65.231 | 44.053 | -7.852 | 1.00 32.99 | AT |
| MOTA | 5821 | 0 | HOH | 222 | 38.789 | 35.275 | 9.625 | 1.00 34.60 | AT |
| ATOM | 5822 | 0 | HOH | 223 | 12.929 | 25.623 | 47.543 | 1.00 32.40 | AT |
| MOTA | 5823 | 0 | HOH | 224 | 74.529 | 33.737 | 18.589 | 1.00 33.85 | ΑT |
| ATOM | 5824 | 0 | HOH | 225 | 16.279 | 43.522 | 36.165 | 1.00 33.82 | ΑT |
| ATOM | 5825 | 0 | HOH | 226 | 13.480 | 14.423 | 55.667 | 1.00 35.36 | AT |
| ATOM | 5826 | 0 | HOH | 227 | 4.656 | 17.272 | 27.720 | 1.00 34.90 | AT |
| ATOM | 5827 | 0 | HOH | 228 | 55.566 | 43.939 | -14.228 | 1.00 37.00 | AT |
| ATOM | 5828 | 0 | HOH | 229 | 18.454 | 21.396 | 68.984 | 1.00 35.96 | AT |
| MOTA | 5829 | 0 | HOH | 230 | 56.014 | 51.348 | -16.697 | 1.00 37.91 | AT |
| ATOM | 5830 | 0 | HOH | 231 | 71.572 | 46.002 | -9.177 | 1.00 36.91 | AT |
| ATOM | 5831 | 0 | HOH | 232 | 39.465 | 30.116 | 20.475 | 1.00 46.92 | AT |
| ATOM | 5832 | 0 | HOH | 233 | 40.113 | 37.155 | 25.795 | 1.00 31.64 | AT |
| MOTA | 5833 | 0 | HOH | 234 | 14.226 | 44.782 | 35.447 | 1.00 33.52 | AT |
| MOTA | 5834 | 0 | HOH | 235 | 20.027 | 45.208 | 30.512 | 1.00 33.92 | AT |
| ATOM | 5835 | 0 | HOH | 236 | 61.895 | 17.484 | 0.210 | 1.00 36.39 | TA |
| ATOM | 5836 | 0 | HOH | 237 | 26.769 | 18.525 | 65.425 | 1.00 33.45 | AT |
| MOTA | 5837 | 0 | HOH | 238 | 30.216 | 49.429 | 23.557 | 1.00 38.87 | AT |
| ATOM | 5838 | 0 | HOH | 239 | 12.005 | 18.680 | 49.514 | 1.00 35.80 | TA |
| ATOM | 5839 | 0 | HOH | 240 | 40.174 | 39.987 | 26.354 | 1.00 36.59 | AT |
| MOTA | 5840 | 0 | HOH | 241 | 19.654 | 14.821 | 28.728 | 1.00 35.91 | AT |
| ATOM | 5841 | 0 | HOH | 242 | 55.447 | 29.046 | 11.959 | 1.00 36.10 | AΤ |
| MOTA | 5842 | 0 | HOH | 243 | 67.323 | 29.753 | -3.238 | 1.00 39.47 | TA |
| ATOM | 5843 | 0 | нон | 244 | 84.687 | 32.541 | 17.389 | 1.00 39.50 | ΑŤ |
| MOTA | 5844 | 0 | HOH | 245 | 54.503 | 28.663 | -6.976 | 1.00 36.28 | AT |
| ATOM | 5845 | 0 | HOH | 246 | 35.636 | 37.561 | 8.625 | 1.00 41.11 | AT |
| ATOM | 5846 | 0 | HOH | 247 | 10.020 | 25.331 | 46.396 | 1.00 38.25 | AT |
| MOTA | 5847 | 0 | HOH | 248 | 11.151 | 27.733 | 14.203 | 1.00 38.20 | ΤA |
| MOTA | 5848 | 0 | HOH | 249 | 10.978 | 20.075 | 53.913 | 1.00 37.44 | TA |
| MOTA | 5849 | 0 | HOH | 250 | 77.340 | 21.792 | 0.783 | 1.00 40.63 | TA |
| MOTA | 5850 | 0 | HOH | 251 | 63.681 | 23.994 | 15.360 | 1.00 37.38 | AT |
| MOTA | 5851 | 0 | HOH | 252 | 11.477 | 23.218 | 48.380 | 1.00 37.57 | AT |
| ATOM | 5852 | 0 | HOH | 253 | 24.484 | 40.133 | 44.556 | 1.00 37.00 | AT |
| ATOM | 5853 | 0 | нон | 254 | 26.870 | 34.997 | 63.642 | 1.00 37.28 | TA |
| ATOM | 5854 | 0 | НОН | 255 | 38.821 | 41.107 | 28.862 | 1.00 37.55 | AT |
| MOTA | 5855 | 0 | нон | 256 | 17.119 | 53.559 | 27.111 | 1.00 35.75 | AT |
| ATOM | 5856 | 0 | нон | 257 | 31.732 | 49.464 | 21.724 | 1.00 40.71 | AT AT |
| ATOM | 5857 | 0 | нон | 258 | 37.233 | 48.595 | 24.778 | 1.00 37.38 | |
| ATOM | 5858 | 0 | HOH | 259 | 64.957 | 31.599 | -4.165 | 1.00 34.72 | AT |
| ATOM | 5859 | 0 | НОН | 260 | 42.059 | 35.767 | 26.985 | 1.00 38.69 | AT AT |
| MOTA | 5860 | 0 | HOH | 261 | 53.170 | 52.497 | -1.737 | 1.00 41.39 1.00 37.27 | AT AT |
| ATOM | 5861 | 0 | HOH | 262 | 15.919 | 8.802 | 51.909 | | AT AT |
| ATOM | 5862 | 0 | HOH | 263 | 60.591 | 34.941 | -9.345 | 1.00 36.16 1.00 38.71 | AT AT |
| MOTA | 5863 | 0 | HOH | 264 | 10.541 | 36.936 | 29.724 21.202 | 1.00 36.97 | AT |
| ATOM | 5864 | 0 | HOH | 265 266 | 31.514 | 44.281 | | 1.00 38.68 | AT |
| ATOM | 5865 | 0 | HOH | 266 | 9.564 | 36.687 33.538 | 51.380 17.348 | 1.00 38.09 | TA |
| ATOM | 5866 | 0 | HOH | 267 | 79.927 | | 11.241 | 1.00 38.09 | AT |
| MOTA | 5867 | 0 | HOH | 268 | 52.604 | 28.637 | 19.676 | 1.00 38.37 | AT |
| MOTA | 5868 | 0 | HOH | 269 | 4.383 | 30.021 | 44.275 | 1.00 37.93 | AT |
| ATOM | 5869 | 0 | HOH | 270 | 39.831 | 37.961 49.901 | -8.433 | 1.00 40.20 | AT |
| ATOM | 5870 | 0 | нон | 271 | 76.908 | 49.901 | -0.433 | 1.00 40.20 | |
| | | | | | | | | | |

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| ATOM | 5871 | 0 | НОН | 272 | 18.828 | 14.845 | 36.392 | 1.00 40.61 | AT |
|------|------|---|-----|-----|----------------|--------|---------|------------|----|
| ATOM | 5872 | 0 | HOH | 273 | 77.377 | 18.239 | 12.575 | 1.00 39.42 | ΑŢ |
| MOTA | 5873 | 0 | HOH | 274 | 51.042 | 29.821 | 13.536 | 1.00 39.59 | AT |
| MOTA | 5874 | 0 | HOH | 275 | 64.107 | 14.629 | 14.266 | 1.00 39.71 | AT |
| ATOM | 5875 | 0 | HOH | 276 | 58.26 7 | 58.162 | -7.799 | 1.00 39.43 | AT |
| MOTA | 5876 | 0 | HOH | 277 | 40.740 | 40.966 | 31.483 | 1.00 40.51 | AT |
| ATOM | 5877 | 0 | HOH | 278 | 15.055 | 10.589 | 55.645 | 1.00 39.15 | AT |
| ATOM | 5878 | 0 | HOH | 279 | 19.789 | 34.347 | 51.860 | 1.00 40.37 | AT |
| MOTA | 5879 | 0 | нон | 280 | 11.976 | 38.727 | 31.710 | 1.00 37.91 | AT |
| MOTA | 5880 | 0 | HOH | 281 | 31.389 | 28.117 | 42.824 | 1.00 40.91 | AT |
| MOTA | 5881 | 0 | нон | 282 | 70.878 | 25.270 | -4.197 | 1.00 43.53 | AΤ |
| ATOM | 5882 | 0 | HOH | 283 | 75.431 | 41.776 | 4.726 | 1.00 40.67 | AT |
| ATOM | 5883 | 0 | HOH | 284 | 62.312 | 53.358 | 28.086 | 1.00 40.98 | AT |
| ATOM | 5884 | 0 | нон | 285 | 62.124 | 59.105 | 9.640 | 1.00 39.55 | AT |
| ATOM | 5885 | 0 | HOH | 286 | 40.707 | 28.142 | 23.532 | 1.00 44.54 | AT |
| MOTA | 5886 | 0 | HOH | 287 | 33.311 | 41.660 | 3.153 | 1.00 41.98 | ΑT |
| MOTA | 5887 | 0 | нон | 288 | 38.680 | 48.495 | 32.258 | 1.00 44.14 | AT |
| ATOM | 5888 | ō | нон | 289 | 32.712 | 38.251 | 44.880 | 1.00 40.32 | AT |
| ATOM | 5889 | ō | нон | 290 | 12.709 | 24.006 | 64.828 | 1.00 40.21 | AT |
| ATOM | 5890 | 0 | нон | 291 | 48.861 | 28.304 | 14.453 | 1.00 42.61 | AT |
| ATOM | 5891 | 0 | нон | 292 | 79.466 | 20.245 | 8.333 | 1.00 40.49 | AT |
| ATOM | 5892 | Ō | нон | 293 | 50.553 | 45.041 | -0.292 | 1.00 42.19 | AT |
| MOTA | 5893 | 0 | нон | 294 | 42.897 | 26.326 | 5.722 | 1.00 41.10 | AT |
| ATOM | 5894 | 0 | нон | 295 | 40.124 | 38.889 | 3.911 | 1.00 42.97 | ΤA |
| ATOM | 5895 | 0 | нон | 296 | -9.725 | 26.259 | 40.147 | 1.00 43.57 | TA |
| ATOM | 5896 | Ō | нон | 297 | 24.463 | 39.296 | 47.536 | 1.00 39.76 | TA |
| ATOM | 5897 | o | нон | 298 | 59.389 | 43.519 | -22.049 | 1.00 45.90 | AT |
| ATOM | 5898 | 0 | нон | 299 | 58.697 | 26.078 | -8.432 | 1.00 42.64 | AT |
| MOTA | 5899 | 0 | HOH | 300 | 59.168 | 23.233 | -8.586 | 1.00 43.13 | AT |
| MOTA | 5900 | 0 | HOH | 301 | 33.173 | 10.853 | 42.976 | 1.00 43.47 | AT |
| ATOM | 5901 | 0 | нон | 302 | 38.135 | 51.041 | 21.685 | 1.00 40.23 | AT |
| MOTA | 5902 | 0 | нон | 303 | 64.003 | 32.204 | 20.781 | 1.00 39.51 | TA |
| ATOM | 5903 | 0 | НОН | 304 | 18.175 | 36.881 | 18.239 | 1.00 42.51 | AT |
| MOTA | 5904 | 0 | нон | 305 | 35.383 | 27.547 | 41.161 | 1.00 46.62 | AT |
| MOTA | 5905 | 0 | HOH | 306 | -1.325 | 41.441 | 28.735 | 1.00 43.36 | AT |
| ATOM | 5906 | 0 | HOH | 307 | 18.409 | 47.629 | 30.260 | 1.00 46.92 | AT |
| ATOM | 5907 | 0 | HOH | 308 | -0.365 | 41.851 | 31.323 | 1.00 43.06 | AT |
| ATOM | 5908 | 0 | HOH | 309 | 31.846 | 13.357 | 43.817 | 1.00 49.55 | TA |
| ATOM | 5909 | 0 | HOH | 310 | 51.910 | 47.621 | -1.442 | 1.00 43.27 | AT |
| ATOM | 5910 | 0 | HOH | 311 | 29.562 | 44.918 | 17.110 | 1.00 52.42 | AT |
| MOTA | 5911 | 0 | HOH | 312 | 30.495 | 43.251 | 13.422 | 1.00 45.47 | AT |
| ATOM | 5912 | 0 | HOH | 313 | 11.474 | 10.744 | 42.423 | 1.00 51.55 | AT |
| ATOM | 5913 | 0 | HOH | 314 | 14.240 | 10.741 | 46.442 | 1.00 43.12 | ΑT |
| ATOM | 5914 | 0 | HOH | 315 | 52.861 | 58.416 | 6.793 | 1.00 44.59 | TA |
| MOTA | 5915 | 0 | HOH | 316 | 28.512 | 44.265 | 22.711 | 1.00 45.20 | AT |
| ATOM | 5916 | 0 | HOH | 317 | 72.643 | 46.339 | -17.391 | 1.00 46.70 | AT |
| MOTA | 5917 | 0 | HOH | 318 | 31.387 | 46.123 | 19.248 | 1.00 43.61 | AT |
| MOTA | 5918 | 0 | HOH | 319 | 78.102 | 45.702 | -8.575 | 1.00 48.47 | AT |
| ATOM | 5919 | 0 | HOH | 320 | 53.628 | 13.801 | 9.167 | 1.00 49.46 | TA |
| ATOM | 5920 | 0 | HOH | 321 | 65.846 | 41.632 | -7.173 | 1.00 44.55 | AT |
| ATOM | 5921 | 0 | HOH | 322 | 41.074 | 48.539 | 27.174 | 1.00 50.50 | ΑT |
| ATOM | 5922 | 0 | HOH | 323 | 30.457 | 41.713 | 20.027 | 1.00 47.21 | AT |
| ATOM | 5923 | 0 | HOH | 324 | 23.888 | 42.661 | 19.783 | | ΑT |
| ATOM | 5924 | 0 | нон | 325 | 46.169 | 56.278 | 15.804 | | AT |
| ATOM | 5925 | 0 | HOH | 326 | 64.632 | 36.604 | -9.385 | | AT |
| ATOM | 5926 | ō | нон | 327 | 50.410 | 48.704 | | | TA |
| ATOM | 5927 | 0 | HOH | 328 | 17.266 | 4.657 | 48.965 | 1.00 55.69 | AT |
| | | | | | | | | | |

| MOTA | 5928 | 0 | HOH | 329 | 15.343 | 49.959 | 36.887 | 1.00 53.08 | AT |
|------|--------------|---|-----|-----|--------|--------|---------|--------------------------|----|
| MOTA | 5929 | 0 | HOH | 330 | 77.778 | 42.870 | 3.924 | 1.00 55.32 | AT |
| MOTA | 5930 | 0 | HOH | 331 | 68.103 | 40.973 | -5.266 | 1.00 57.57 | AT |
| ATOM | 5931 | 0 | HOH | 332 | 21.493 | 20.139 | 67.130 | 1.00 33.16 | ΑT |
| ATOM | 5932 | 0 | HOH | 333 | 81.269 | 24.355 | 14.982 | 1.00 33.69 | AT |
| ATOM | 5933 | 0 | HOH | 334 | -5.903 | 30.538 | 26.686 | 1.00 40.35 | AT |
| ATOM | 5934 | 0 | HOH | 335 | 80.030 | 32.515 | -0.810 | 1.00 39.92 | AT |
| MOTA | 5935 | 0 | HOH | 336 | -7.205 | 27.318 | 42.127 | 1.00 37.50 | AT |
| MOTA | 5936 | 0 | HOH | 337 | 0.251 | 35.076 | 40.556 | 1.00 41.65 | AT |
| ATOM | 5937 | 0 | HOH | 338 | 67.263 | | -10.701 | 1.00 34.16 | AT |
| ATOM | 5938 | ō | НОН | 339 | 78.930 | 41.885 | 0.871 | 1.00 36.88 | AT |
| ATOM | 5939 | ō | нон | 340 | 81.589 | 22.534 | 9.006 | 1.00 32.20 | AT |
| ATOM | 5940 | ō | нон | 341 | -4.841 | 30.109 | 35.827 | 1.00 39.55 | AT |
| ATOM | 5941 | Ö | нон | 342 | 24.216 | 28.828 | 53.120 | 1.00 48.54 | AT |
| MOTA | 5942 | o | нон | 343 | 58.172 | | -15.457 | 1.00 43.54 | AT |
| ATOM | 5943 | Ö | НОН | 344 | 72.009 | | -12.680 | 1.00 44.56 | AT |
| ATOM | 5944 | 0 | HOH | 345 | 70.243 | | -16.741 | 1.00 37.48 | TA |
| MOTA | 5945 | 0 | НОН | 346 | 63.182 | | -22.683 | 1.00 47.83 | TA |
| ATOM | 5946 | 0 | HOH | 347 | 59.201 | | -12.511 | 1.00 48.60 | TA |
| ATOM | 5947 | 0 | HOH | 348 | 73.024 | 32.150 | -12.311 | 1.00 48.80 | AT |
| | | | | | | | 55.406 | | |
| ATOM | 5948 | 0 | HOH | 349 | 36.241 | 17.553 | 33.327 | 1.00 43.52 1.00 44.23 | AT |
| MOTA | 5949 | 0 | HOH | 351 | 14.204 | 56.480 | | | AT |
| ATOM | 5950 | 0 | HOH | 352 | 81.607 | 27.771 | 10.204 | 1.00 46.37 | AT |
| ATOM | 5951 | 0 | нон | 353 | 72.230 | 29.150 | -2.863 | 1.00 44.64 | AT |
| ATOM | 5952 | 0 | нон | 354 | 63.965 | 35.398 | | 1.00 40.75 | TA |
| ATOM | 5953 | 0 | HOH | 355 | 83.662 | 27.262 | 2.560 | 1.00 52.07 | AT |
| MOTA | 5954 | 0 | HOH | 356 | 54.821 | 57.411 | -7.143 | 1.00 47.42 | AT |
| MOTA | 5955 | 0 | HOH | 357 | 75.827 | 24.345 | -2.592 | 1.00 38.53 | AT |
| ATOM | 5956 | 0 | HOH | 358 | -3.100 | 29.989 | 33.712 | 1.00 35.26 | AT |
| ATOM | 5957 | 0 | нон | 359 | 76.580 | 32.031 | 17.038 | 1.00 45.16 | TA |
| ATOM | 5958 | 0 | HOH | 360 | 61.004 | 63,374 | -0.717 | 1.00 51.75 | AT |
| ATOM | 5959 | 0 | нон | 361 | 57.555 | | -17.566 | 1.00 37.15 | AT |
| MOTA | 5960 | 0 | HOH | 362 | 46.758 | 41.005 | -9.571 | 1.00 49.08 | AT |
| MOTA | 5961 | 0 | HOH | 363 | 65.046 | 41.921 | 10.931 | 1.00 43.73 | AT |
| MOTA | 5962 | 0 | HOH | 364 | 60.495 | | -20.999 | 1.00 39.43 | AT |
| ATOM | 5963 | 0 | нон | 365 | 24.639 | 46.742 | 50.064 | 1.00 49.54 | TA |
| ATOM | 5964 | 0 | HOH | 366 | 65.360 | | -12.244 | 1.00 42.08 | AT |
| ATOM | 5965 | 0 | HOH | 367 | 81.253 | 38.379 | 6.191 | 1.00 44.60 | AT |
| MOTA | 5966 | 0 | HOH | 368 | 20.278 | 58.789 | 32.999 | 1.00 51.96 | AT |
| MOTA | 5967 | 0 | HOH | 369 | 35.754 | 25.608 | 43.846 | 1.00 41.69 | AΤ |
| MOTA | 5968 | 0 | HOH | 370 | 58.812 | 30.456 | 20.182 | 1.00 47.60 | AT |
| ATOM | 5969 | 0 | HOH | 371 | 62.070 | | -12.130 | 1.00 38.66 | TA |
| ATOM | 5970 | 0 | HOH | 372 | 28.704 | 57.271 | 37.789 | 1.00 53.91 | AT |
| MOTA | 5971 | 0 | HOH | 373 | 16.768 | 31.252 | 63.214 | 1.00 43.22 | AT |
| MOTA | 5972 | 0 | HOH | 374 | 17.431 | 24.978 | 67.168 | 1.00 45.45 | AT |
| MOTA | 5973 | 0 | HOH | 375 | 51.911 | 28.483 | -4.087 | 1.00 57.67 | AT |
| MOTA | 5974 | 0 | HOH | 376 | 61.859 | 13.653 | 15.354 | 1.00 48.16 | AT |
| ATOM | 597 5 | 0 | HOH | 377 | 60.309 | 37.228 | -7.635 | 1.00 40.72 | AT |
| ATOM | 5976 | 0 | HOH | 378 | 76.341 | 49.000 | 11.927 | 1.00 51.08 | TA |
| ATOM | 59 77 | 0 | HOH | 379 | 26.911 | 4.583 | 49.436 | 1.00 50.11 | AT |
| ATOM | 5978 | 0 | нон | 380 | 60.796 | 28.003 | | 1.00 41.08 | AT |
| MOTA | 5979 | 0 | HOH | 381 | 64.912 | 34.210 | | 1.00 54.13 | AT |
| ATOM | 5980 | ō | нон | 382 | 24.406 | 25.422 | | 1.00 46.00 | AT |
| ATOM | 5981 | 0 | нон | 383 | 27.206 | 10.460 | | 1.00 48.67 | AT |
| ATOM | 5982 | ō | нон | 384 | 69.870 | 64.847 | | 1.00 51.86 | TA |
| ATOM | 5983 | Ö | нон | 385 | 13.388 | 53.599 | | 1.00 53.21 | AT |
| ATOM | 5984 | Ö | нон | 386 | 65.207 | | -23.032 | 1.00 44.87 | AT |
| AION | 2204 | • | | 200 | 33.207 | | | | |

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| MOTA | 5985 | 0 | нон | 387 | 23.812 | 43.965 | 31.871 | 1.00 51.01 | AT |
|------|------|---|-----|-----|--------|--------|---------|------------|----|
| MOTA | 5986 | 0 | HOH | 388 | 27.925 | 56,723 | 25.402 | 1.00 50.91 | AT |
| ATOM | 5987 | 0 | HOH | 389 | 22.429 | 53.122 | 37.372 | 1.00 40.24 | AT |
| ATOM | 5988 | 0 | HOH | 390 | 20.340 | 37.818 | 64.894 | 1.00 43.91 | AT |
| ATOM | 5989 | 0 | HOH | 391 | 3.772 | 17.279 | 18.046 | 1.00 55.83 | AT |
| MOTA | 5990 | 0 | HOH | 392 | 61.560 | 29.447 | -8.011 | 1.00 48.85 | TA |
| MOTA | 5991 | 0 | HOH | 393 | 40.737 | 49.676 | 12.185 | 1.00 48.28 | AT |
| MOTA | 5992 | 0 | HOH | 394 | 47.566 | 44.388 | 26.446 | 1.00 47.81 | AT |
| MOTA | 5993 | 0 | HOH | 395 | 62.091 | 37.019 | 27.629 | 1.00 53.63 | AT |
| ATOM | 5994 | 0 | HOH | 396 | 45.170 | 49.972 | 14.734 | 1.00 52.56 | AT |
| ATOM | 5995 | 0 | HOH | 397 | 25.713 | 56.378 | 37.487 | 1.00 46.30 | ΑT |
| ATOM | 5996 | 0 | HOH | 398 | 19.430 | 54.171 | 39.827 | 1.00 43.81 | AT |
| ATOM | 5997 | 0 | HOH | 399 | 25.461 | 13.937 | 28.867 | 1.00 46.75 | AT |
| MOTA | 5998 | 0 | нон | 400 | 65.078 | 42.400 | 27.343 | 1.00 58.24 | AT |
| ATOM | 5999 | 0 | HOH | 401 | 15.750 | 35.665 | 16.140 | 1.00 49.43 | AT |
| MOTA | 6000 | 0 | HOH | 402 | 30.823 | 49.012 | 9.778 | 1.00 49.25 | AT |
| ATOM | 6001 | 0 | нон | 403 | 63.642 | 30.868 | -6.737 | 1.00 63.10 | AT |
| ATOM | 6002 | 0 | HOH | 404 | -5.102 | 30.693 | 29.722 | 1.00 44.38 | AT |
| ATOM | 6003 | 0 | HOH | 405 | 5.998 | 28.463 | 48.599 | 1.00 45.41 | AT |
| ATOM | 6004 | 0 | нон | 406 | 78.918 | 22,759 | 14.469 | 1.00 48.83 | AT |
| MOTA | 6005 | 0 | нон | 407 | 67.800 | 14.615 | -0.774 | 1.00 47.19 | AT |
| ATOM | 6006 | 0 | HOH | 408 | -8.454 | 30.970 | 25.750 | 1.00 52.46 | AT |
| ATOM | 6007 | 0 | HOH | 409 | 39.982 | 27.102 | 31.435 | 1.00 51.86 | AT |
| ATOM | 6008 | 0 | нон | 410 | 73.123 | 40.475 | 21.437 | 1.00 60.13 | TA |
| MOTA | 6009 | 0 | нон | 411 | 60.888 | 14.040 | 1.887 | 1.00 46.41 | AT |
| ATOM | 6010 | 0 | HOH | 412 | 36.503 | 50.699 | 10.642 | 1.00 54.16 | AT |
| MOTA | 6011 | 0 | нон | 413 | 59.362 | 62.211 | -6.530 | 1.00 49.09 | AT |
| ATOM | 6012 | 0 | нон | 414 | 28.103 | 13.240 | 52.474 | 1.00 47.88 | AT |
| ATOM | 6013 | 0 | HOH | 415 | 32.010 | 21.506 | 60.871 | 1.00 51.04 | AT |
| ATOM | 6014 | 0 | HOH | 416 | 35.534 | 13.760 | 51.867 | 1.00 48.76 | AT |
| MOTA | 6015 | 0 | HOH | 417 | 40.198 | 51.587 | 23.313 | 1.00 47.59 | AT |
| ATOM | 6016 | 0 | HOH | 418 | 32.582 | 27.322 | 18.391 | 1.00 59.17 | AT |
| MOTA | 6017 | 0 | HOH | 419 | 70.979 | 43.580 | -23.023 | 1.00 62.55 | AT |
| MOTA | 6018 | 0 | HOH | 420 | 72.711 | 52.348 | -21.252 | 1.00 55.53 | AT |
| MOTA | 6019 | 0 | HOH | 421 | 51.501 | 60.903 | 2.181 | 1.00 56.42 | AT |
| ATOM | 6020 | 0 | HOH | 423 | 53.460 | 21.733 | -0.240 | 1.00 63.43 | TA |
| ATOM | 6021 | 0 | HOH | 424 | 55.865 | 19.944 | -0.930 | 1.00 45.43 | TA |
| ATOM | 6022 | 0 | HOH | 425 | 11.457 | 18.171 | 63.981 | 1.00 40.96 | AT |
| MOTA | 6023 | 0 | HOH | 426 | 29.667 | 28.514 | 52.029 | 1.00 40.86 | AT |
| MOTA | 6024 | 0 | HOH | 427 | 21.382 | 43.057 | 31.379 | 1.00 37.88 | AT |
| ATOM | 6025 | 0 | HOH | 428 | 72.431 | 56.442 | -14.816 | 1.00 38.78 | AT |
| MOTA | 6026 | 0 | HOH | 429 | 13.645 | 35.387 | 57.232 | 1.00 45.75 | TA |
| ATOM | 6027 | 0 | HOH | 430 | 47.325 | 44.655 | 9.515 | 1.00 52.79 | AT |
| MOTA | 6028 | 0 | HOH | 431 | 12.413 | 9.161 | 45.090 | 1.00 53.71 | AT |
| MOTA | 6029 | 0 | HOH | 432 | 69.847 | 39.107 | -2.341 | 1.00 47.46 | AT |
| MOTA | 6030 | 0 | HOH | 433 | 40.580 | 34.476 | 3.546 | 1.00 42.74 | AT |
| MOTA | 6031 | 0 | HOH | 434 | 68.590 | 27.199 | -5.061 | 1.00 50.14 | ΑT |
| ATOM | 6032 | 0 | HOH | 435 | 81.709 | 33.738 | 20.448 | 1.00 51.49 | TA |
| ATOM | 6033 | 0 | HOH | 436 | 21.276 | 6.862 | 53.221 | 1.00 43.81 | TA |
| ATOM | 6034 | 0 | HOH | 437 | 63.959 | 28.541 | 24.084 | 1.00 48.89 | AT |
| ATOM | 6035 | 0 | HOH | 438 | 44.540 | 42.464 | 26.796 | 1.00 45.92 | AT |
| MOTA | 6036 | 0 | HOH | 439 | 26.430 | 12.510 | | 1.00 41.22 | AT |
| ATOM | 6037 | 0 | HOH | 440 | 13.505 | 42.803 | | 1.00 49.02 | AT |
| ATOM | 6038 | 0 | HOH | 441 | 61.236 | 27.483 | | 1.00 53.99 | TA |
| ATOM | 6039 | 0 | HOH | 442 | 48.452 | 32.235 | | 1.00 39.84 | AT |
| ATOM | 6040 | 0 | HOH | 443 | -6.734 | 17.777 | | 1.00 43.66 | AT |
| MOTA | 6041 | 0 | HOH | 444 | 68.689 | 11.054 | 1.803 | 1.00 54.43 | AT |
| | | | | | | | | | |

| 3 TOM | C043 | ^ | TIOIT | 445 | 64 333 | 0 100 | 7 000 | | |
|-------|------------------|----|-------|-----|--------|--------|--------|------------|------------------------|
| ATOM | 6042 | 0 | нон | 445 | 64.733 | 8.182 | 7.092 | 1.00 51.11 | AT |
| MOTA | 6043 | 0 | HOH | 446 | 47.452 | 47.307 | 25.789 | 1.00 50.83 | AT |
| ATOM | 6044 | O | HOH | 447 | -5.597 | 17.191 | 22.022 | 1.00 62.54 | AT |
| ATOM | 6045 | 0 | HOH | 448 | 34.703 | 54.274 | 40.793 | 1.00 43.46 | TA |
| ATOM | 6046 | 0 | HOH | 449 | 7.584 | 42.423 | 41.797 | 1.00 50.29 | AT |
| ATOM | 6047 | 0 | HOH | 450 | 68.745 | 9.611 | 12.516 | 1.00 44.55 | AT |
| ATOM | 6048 | 0 | НОН | 451 | 10.345 | 30.448 | 14.624 | 1.00 52.09 | AT |
| | | | | 452 | | | | | |
| ATOM | 6049 | 0 | нон | | 28.739 | 24.654 | 67.367 | 1.00 43.81 | TA |
| ATOM | 6050 | 0 | HOH | 453 | 59.859 | 15.451 | -0.538 | 1.00 50.23 | TA |
| MOTA | 6051 | 0 | нон | 454 | 9.715 | 22.615 | 40.260 | 1.00 55.68 | TA |
| MOTA | 6052 | 0 | HOH | 455 | 8.408 | 33.305 | 58.554 | 1.00 48.77 | AT |
| MOTA | 6053 | 0 | HOH | 456 | 82.808 | 20.346 | 7.688 | 1.00 64.19 | AT |
| MOTA | 6054 | 0 | HOH | 457 | 20.676 | 9.525 | 40.046 | 1.00 47.64 | AT |
| MOTA | 6055 | 0 | HOH | 458 | 12.300 | 21.911 | 45.521 | 1.00 55.95 | AT |
| ATOM | 6056 | Ō | нон | 459 | 12.849 | 37.059 | 54.956 | 1.00 47.15 | AT |
| ATOM | | 0 | | 460 | | 37.315 | | | |
| | 6057 | | HOH | | 18.947 | | 56.296 | 1.00 55.87 | AT |
| ATOM | 6058 | 0 | нон | 461 | 42.279 | 43.046 | 32.215 | 1.00 55.34 | AT |
| ATOM | 6059 | 0 | HOH | 462 | 58.113 | 60.078 | -9.775 | 1.00 41.21 | AT |
| ATOM | 6060 | 0 | HOH | 463 | -4.882 | 24.186 | 43.569 | 1.00 49.34 | AT |
| MOTA | 6061 | 0 | HOH | 464 | 2.275 | 30.894 | 44.638 | 1.00 49.59 | AT |
| ATOM | 6062 | 0 | HOH | 465 | 11.908 | 42.581 | 46.538 | 1.00 54.17 | $\mathtt{T}\mathtt{A}$ |
| ATOM | 6063 | 0 | HOH | 466 | 25.196 | 30.973 | 68.678 | 1.00 54.36 | TA |
| ATOM | 6064 | 0 | HOH | 467 | 55.729 | 18.620 | -3.586 | 1.00 51.13 | AT |
| ATOM | 6065 | Ō | HOH | 468 | 12.016 | 5.491 | 40.550 | 1.00 54.15 | AT |
| ATOM | 6066 | 0 | нон | 469 | 56.711 | 29.214 | 27.406 | 1.00 63.41 | AT |
| MOTA | 6067 | Ö | нон | 470 | 56.150 | 18.575 | 3.127 | 1.00 57.43 | AT |
| | | | | | 18.186 | | | | |
| MOTA | 6068 | 0 | HOH | 471 | | 11.646 | 26.302 | 1.00 54.34 | AT |
| ATOM | 6069 | S1 | DTT | 1 | 74.181 | 38.187 | -0.498 | 1.00 67.01 | TT1 |
| MOTA | 6070 | Cl | TTC | 1 | 72.670 | 38.130 | -1.524 | 1.00 67.92 | TT1 |
| ATOM | 6071 | C2 | DTT | 1 | 72.656 | 36.968 | -2.590 | 1.00 68.22 | TTI |
| MOTA | 6072 | 02 | DTT | 1 | 71.393 | 37.023 | -3.311 | 1.00 68.98 | TT1 |
| ATOM | 6073 | C3 | DTT | 1 | 73.769 | 37.036 | -3.768 | 1.00 67.93 | TT1 |
| MOTA | 6074 | 03 | DTT | 1 | 73.674 | 35.873 | -4.701 | 1.00 67.85 | TT1 |
| ATOM | 6075 | C4 | DTT | 1, | 75.213 | 37.003 | -3.287 | 1.00 67.57 | TT1 |
| ATOM | 6076 | S4 | DTT | 1 | 75.541 | 38.418 | -2.099 | 1.00 67.52 | TTl |
| ATOM | 6077 | S1 | DTT | 2 | 54.935 | 53.026 | 7.820 | 1.00 53.56 | TT2 |
| ATOM | 6078 | Cl | DTT | 2 | 53.759 | 51.637 | 7.760 | 1.00 53.84 | TT2 |
| | 6079 | | DTT | 2 | 52.738 | 51.710 | 6.562 | 1.00 54.90 | TT2 |
| MOTA | | C2 | | | | | | 1.00 54.30 | |
| MOTA | 6080 | 02 | DTT | 2 | 51.885 | 50.534 | 6.613 | | TT2 |
| MOTA | 6081 | C3 | TTC | 2 | 51.681 | 52.940 | 6.568 | 1.00 54.93 | TT2 |
| MOTA | 6082 | 03 | DTT | 2 | 50.780 | 52.918 | 5.376 | 1.00 55.43 | TT2 |
| ATOM | 6083 | C4 | DTT | 2 | 52.313 | 54.325 | 6.524 | 1.00 54.51 | TT2 |
| MOTA | 6084 | S4 | DTT | 2 | 53.485 | 54.549 | 7.971 | 1.00 54.25 | TT2 |
| ATOM | 6085 | S1 | DTT | 3 | 9.841 | 19.197 | 19.765 | 1.00 46.94 | TT3 |
| ATOM | 6086 | C1 | DTT | 3 | 8.080 | 19.681 | 19.855 | 1.00 44.23 | TT3 |
| ATOM | 6087 | C2 | DTT | 3 | 7.123 | 18.477 | 20.203 | 1.00 45.91 | TT3 |
| ATOM | 6088 | 02 | DTT | 3 | 5.758 | 18.968 | 20.283 | 1.00 45.68 | TT3 |
| ATOM | 6089 | C3 | DTT | 3 | 7.023 | 17.285 | 19.113 | 1.00 46.42 | TT3 |
| | | | | | | | 19.567 | 1.00 49.11 | TT3 |
| ATOM | 6090 | 03 | DTT | 3 | 6.110 | 16.195 | | | |
| ATOM | 6091 | C4 | DTT | 3 | 8.337 | 16.568 | 18.812 | 1.00 45.21 | TT3 |
| MOTA | 6092 | S4 | DTT | 3 | 9.629 | 17.785 | 18.211 | 1.00 44.44 | TT3 |
| MOTA | 6093 | S1 | DTT | 4 | 19.785 | 34.825 | 23.721 | 1.00 49.21 | TT4 |
| MOTA | 6094 | C1 | DTT | 4 | 19.784 | 36.095 | 25.038 | 1.00 49.59 | TT4 |
| MOTA | 6095 | C2 | TTC | 4 | 18.556 | 37.084 | 24.993 | 1.00 51.01 | TT4 |
| ATOM | 609 6 | 02 | TTG | 4 | 18.673 | 38.019 | 26.105 | 1.00 52.92 | TT4 |
| ATOM | 6097 | C3 | DTT | 4 | 18.440 | 38.051 | 23.699 | 1.00 50.89 | TT4 |
| ATOM | 6098 | 03 | DTT | 4 | 17.234 | 38.926 | 23.759 | 1.00 51.66 | TT4 |
| | 5555 | | | • | | 55.520 | | | |

| MOTA | 6099 | C4 | TTG | 4 | 18.302 | 37.325 | 22.365 | 1.00 50.07 | TT4 |
|------|------|------|-----|----|--------|--------|---------|------------|-----|
| MOTA | 6100 | S4 | DTT | 4 | 19.750 | 36.164 | 22.087 | 1.00 49.50 | 774 |
| ATOM | 6101 | S1 | DTT | 5 | 13.883 | 15.968 | 40.130 | 1.00 53.89 | TT5 |
| ATOM | 6102 | Cl | DTT | 5 | 12.694 | 17.323 | 39.827 | 1.00 54.86 | TT5 |
| MOTA | 6103 | C2 | DTT | 5 | 11.608 | 17.502 | 40.955 | 1.00 55.83 | TT5 |
| ATOM | 6104 | 02 | DTT | 5 | 10.754 | 18.625 | 40.590 | 1.00 57.35 | TT5 |
| MOTA | 6105 | C3 | DTT | 5 | 10.561 | 16.283 | 41.172 | 1.00 55.92 | TTS |
| ATOM | 6106 | 03 | DTT | 5 | 9.597 | 16.559 | 42.278 | 1.00 56.47 | TT5 |
| MOTA | 6107 | C4 | DTT | 5 | 11.194 | 14.953 | 41.564 | 1.00 55.56 | TT5 |
| ATOM | 6108 | S4 | DTT | 5 | 12.443 | 14.418 | 40.274 | 1.00 55.31 | TT5 |
| ATOM | 6109 | Cl | GOL | 6 | 25.840 | 30.485 | 23.369 | 1.00 60.12 | OL1 |
| ATOM | 6110 | 01 | GOL | 6 | 24.418 | 30.344 | 23.510 | 1.00 58.37 | OL1 |
| ATOM | 6111 | C2 | GOL | 6 | 26.254 | 30.565 | 21.841 | 1.00 60.62 | OL1 |
| MOTA | 6112 | 02 | GOL | 6 | 26.921 | 31.825 | 21.610 | 1.00 61.53 | OL1 |
| MOTA | 6113 | C3 | GOL | 6 | 25.019 | 30.470 | 20.890 | 1.00 60.48 | OL1 |
| ATOM | 6114 | 03 | GOL | 6 | 25.353 | 30.640 | 19.507 | 1.00 60.02 | OL1 |
| ATOM | 6115 | C1 | GOL | 7 | 79.028 | 22.813 | 10.783 | 1.00 59.60 | OL2 |
| ATOM | 6116 | 01 | GOL | 7 | 78.201 | 22.510 | 11.912 | 1.00 61.71 | OL2 |
| ATOM | 6117 | C2 | GOL | 7 | 79.615 | 24.278 | 10.893 | 1.00 59.54 | OL2 |
| MOTA | 6118 | 02 | GOL | 7 | 81.057 | 24.201 | 10.902 | 1.00 59.72 | OL2 |
| ATOM | 6119 | C3 | GOL | 7 | 79.147 | 25.010 | 12.189 | 1.00 58.44 | OL2 |
| ATOM | 6120 | 03 | GOL | 7 | 79.958 | 26.145 | 12.514 | 1.00 56.91 | OL2 |
| ATOM | | NA+1 | NA1 | 1 | 63.339 | 31.566 | -2.590 | 1.00 26.24 | ONS |
| MOTA | 6122 | NA+1 | NA1 | 2 | 65.507 | 33.113 | 17.476 | 1.00 24.78 | ONS |
| ATOM | 6123 | NA+1 | NAl | 3 | 52.138 | 43.339 | -0.467 | 1.00 31.32 | ONS |
| ATOM | | NA+1 | | 4 | 11.564 | 27.003 | 46.250 | 1.00 28.57 | ONS |
| MOTA | 6125 | NA+1 | NAl | 5 | 22.858 | 38.903 | 45.868 | 1.00 35.79 | ONS |
| ATOM | 6126 | NA+1 | NAl | 6 | 12.049 | 37.399 | 33.606 | 1.00 30.07 | ONS |
| ATOM | 6127 | NA+1 | NA1 | 7 | 52.399 | 30.404 | 9.576 | 1.00 28.65 | ONS |
| ATOM | 6128 | NA+1 | NA1 | 8 | 61.322 | 58.273 | -12.969 | 1.00 38.12 | ONS |
| MOTA | 6129 | CL-1 | CL1 | 9 | 74.315 | 48.004 | -8.768 | 1.00 36.69 | ONS |
| ATOM | 6130 | CL-1 | CL1 | 10 | 10.448 | 28.591 | 48.519 | 1.00 26.89 | ONS |
| MOTA | 6131 | CL-1 | CL1 | 11 | 49.897 | 29.847 | 8.163 | 1.00 28.28 | ONS |
| MOTA | 6132 | CL-1 | CL1 | 12 | 68.370 | 32.685 | 17.763 | 1.00 30.08 | ONS |
| ATOM | 6133 | CL-1 | CL1 | 13 | 21.352 | 41.348 | 46.322 | 1.00 33.00 | ONS |
| ATOM | 6134 | CL-1 | CL1 | 14 | 21.514 | 34.817 | 28.080 | 1.00 20.85 | ONS |
| ATOM | 6135 | CL-1 | CL1 | 15 | 70.235 | 40.020 | 0.588 | 1.00 21.12 | ONS |
| ATOM | 6136 | CL-1 | CL1 | 16 | 55.303 | 48.583 | 9.136 | 1.00 22.36 | ONS |
| MOTA | 6137 | CL-1 | CLl | 17 | 61.816 | 29.359 | -3.630 | 1.00 27.78 | ONS |
| ATOM | 6138 | CL-1 | CLl | 18 | 66.265 | 35.653 | 18.338 | 1.00 26.36 | ONS |
| ATOM | 6139 | CL-1 | CL1 | 19 | 9.405 | 38.244 | 34.766 | 1.00 27.56 | ONS |
| ATOM | 6140 | CL-1 | CL1 | 20 | 56.075 | 30.580 | -5.205 | 1.00 30.76 | ONS |
| ATOM | 6141 | CL-1 | CL1 | 21 | 51.184 | 42.277 | -2.989 | 1.00 29.31 | ONS |
| ATOM | 6142 | CL-1 | CL1 | 22 | 8.488 | 34.106 | 46.950 | 1.00 31.69 | ONS |
| MOTA | 6143 | CL-1 | CL1 | 23 | 26.255 | 30.563 | 26.909 | 1.00 29.29 | ONS |
| MOTA | 6144 | CL-1 | CL1 | 24 | 14.532 | 19.865 | 38.018 | 1.00 22.44 | ONS |
| MOTA | | CL-1 | | 25 | 38.459 | 48.451 | | 1.00 41.86 | ONS |
| ATOM | 6146 | CL-1 | CL1 | 26 | 48.969 | 36.502 | | | ONS |
| MOTA | 6147 | CL-1 | CL1 | 27 | 19.241 | 17.587 | 34.034 | 1.00 29.08 | ONS |
| END | | | | | | | | | |
| | | | | | | | | | |

Figure 2

| | | Atom | | | | | _ | , | |
|------|---|------|------|---|------------|-------|--------|--------------|----------------------|
| | | Type | Res. | | - <u>X</u> | Y | Z | OCC B | MOL |
| MOTA | 1 | C | GLY | 1 | 3.531 | 2.676 | 31.918 | 1.00 23.54 | ACPS |
| ATOM | 2 | 0 | GLY | 1 | 2.877 | 3.712 | 32.042 | 1.00 24.07 | ACPS |
| MOTA | 3 | N | GLY | 1 | 3.058 | 2.705 | 29.459 | 1.00 25.97 | · · · · - |
| ATOM | 4 | CA | GLY | 1 | 3.503 | 1.884 | 30.623 | 1.00 24.19 | ACPS |
| MOTA | 5 | N | ILE | 2 | 4.299 | 2.191 | 32.884 | 1.00 21.88 | ACPS |
| ATOM | 6 | CA | ILE | 2 | 4.396 | 2.857 | 34.180 | 1.00 20.22 | ACPS |
| ATOM | 7 | CB | ILE | 2 | 4.119 | 1.857 | 35.329 | 1.00 20.22 | ACPS |
| ATOM | 8 | CG2 | ILE | 2 | 4.474 | 2.485 | 36.679 | - | ACPS |
| ATOM | 9 | CG1 | | 2 | | | | 1.00 18.46 | ACPS |
| | _ | CGI | 7112 | 4 | 2.647 | 1.429 | 35.289 | 1.00 19.13 | ACPS |

| MOTA | 10 | CD1 | ILE | 2 | 2.303 | 0.294 | 36.250 | 1.00 20.56 | ACPS |
|------|----|-----|-----|----|----------------|--------|----------------|------------|------|
| MOTA | 11 | С | ILE | 2 | 5.769 | 3.490 | 34.376 | 1.00 19.58 | ACPS |
| MOTA | 12 | 0 | ILE | 2 | 6.798 | 2.827 | 34.223 | 1.00 19.75 | ACPS |
| MOTA | 13 | N | TYR | 3 | 5.779 | 4.780 | 34.704 | 1.00 18.83 | ACPS |
| ATOM | 14 | CA | TYR | 3 | 7.024 | 5.493 | 34.942 | 1.00 18.94 | ACPS |
| MOTA | 15 | CB | TYR | 3 | 6.814 | 7.004 | 34.809 | 1.00 21.16 | ACPS |
| ATOM | 16 | CG | TYR | 3 | 8.059 | 7.808 | 35.103 | 1.00 23.30 | ACPS |
| ATOM | 17 | CD1 | TYR | 3 | 9.164 | 7.761 | 34.246 | 1.00 24.81 | ACPS |
| MOTA | 18 | CE1 | TYR | 3 | 10.326 | 8.486 | 34.525 | 1.00 25.94 | ACPS |
| ATOM | 19 | CD2 | TYR | 3 | 8.145 | 8.601 | 36.246 | 1.00 24.18 | ACPS |
| ATOM | 20 | CE2 | TYR | 3 | 9.297 | 9.329 | 36.534 | 1.00 25.63 | ACPS |
| ATOM | 21 | CZ | TYR | 3 | 10.384 | 9.267 | 35.672 | 1.00 26.92 | ACPS |
| ATOM | 22 | OH | TYR | 3 | 11.524 | 9.974 | 35.970 | 1.00 28.98 | ACPS |
| MOTA | 23 | C | TYR | 3 | 7.555 | 5.165 | 36.340 | 1.00 17.87 | ACPS |
| MOTA | 24 | 0 | TYR | 3 | 8.757 | 4.968 | 36.525 | 1.00 18.51 | ACPS |
| ATOM | 25 | N | GLY | 4 | 6.657 | 5.107 | 37.325 | 1.00 16.17 | ACPS |
| MOTA | 26 | CA | GLY | 4 | 7.088 | 4.789 | 38.678 | 1.00 13.94 | ACPS |
| ATOM | 27 | C | GLY | 4 | 5.937 | 4.643 | 39.657 | 1.00 13.19 | ACPS |
| ATOM | 28 | 0 | GLY | 4 | 4.819 | 5.094 | 39.38 7 | 1.00 13.25 | ACPS |
| ATOM | 29 | N | ILE | 5 | 6.217 | 4.001 | 40.794 | 1.00 12.43 | ACPS |
| ATOM | 30 | CA | ILE | 5 | 5.209 | 3.822 | 41.841 | 1.00 11.10 | ACPS |
| ATOM | 31 | CB | ILE | 5 | 4.718 | 2.326 | 41.963 | 1.00 11.22 | ACPS |
| ATOM | 32 | CG2 | ILE | 5 | 4.330 | 1.793 | 40.572 | 1.00 12.21 | ACPS |
| ATOM | 33 | CG1 | ILE | 5 | 5.785 | 1.441 | 42.619 | 1.00 11.21 | ACPS |
| MOTA | 34 | CD1 | ILE | 5 | 5.338 | -0.010 | 42.831 | 1.00 12.31 | ACPS |
| MOTA | 35 | C | ILE | 5 | 5 .7 93 | 4.294 | 43.175 | 1.00 10.72 | ACPS |
| MOTA | 36 | 0 | ILE | 5 | 7.013 | 4.358 | 43.346 | 1.00 11.21 | ACPS |
| MOTA | 37 | N | GLY | 6 | 4.910 | 4.644 | 44.108 | 1.00 10.20 | ACPS |
| ATOM | 38 | CA | GLY | 6 | 5.347 | 5.102 | 45.414 | 1.00 9.68 | ACPS |
| MOTA | 39 | C | GLY | 6 | 4.348 | 4.762 | 46.503 | 1.00 10.17 | ACPS |
| ATOM | 40 | 0 | GLY | 6 | 3.139 | 4.776 | 46.261 | 1.00 9.96 | ACPS |
| MOTA | 41 | N | LEU | 7 | 4.859 | 4.459 | 47.697 | 1.00 9.09 | ACPS |
| MOTA | 42 | CA | LEU | 7 | 4.024 | 4.109 | 48.852 | 1.00 9.72 | ACPS |
| MOTA | 43 | CB | LEU | 7 | 4.058 | 2.588 | 49.078 | 1.00 10.10 | ACPS |
| ATOM | 44 | CG | LEU | 7 | 3.308 | 2.001 | 50.285 | 1.00 9.72 | ACPS |
| ATOM | 45 | | LEU | 7 | 1.814 | 2.059 | 50.037 | 1.00 12.07 | ACPS |
| ATOM | 46 | | LEU | 7 | 3.741 | 0.552 | 50.503 | 1.00 10.42 | ACPS |
| MOTA | 47 | C | LEU | 7 | 4.530 | 4.804 | 50.121 | 1.00 10.28 | ACPS |
| MOTA | 48 | 0 | LEU | 7 | 5. 7 39 | 4.936 | 50.319 | 1.00 10.25 | ACPS |
| ATOM | 49 | N | ASP | 8 | 3.610 | 5.255 | 50.976 | 1.00 9.98 | ACPS |
| ATOM | 50 | CA | ASP | 8 | 4.024 | 5.871 | 52.230 | 1.00 9.91 | ACPS |
| MOTA | 51 | CB | ASP | 8 | 4.323 | 7.365 | 52.045 | 1.00 9.85 | ACPS |
| ATOM | 52 | CG | ASP | 8 | 5.223 | 7.887 | 53.128 | 1.00 11.38 | ACPS |
| ATOM | 53 | | ASP | 8 | 4.723 | 8.465 | 54.110 | 1.00 12.14 | ACPS |
| MOTA | 54 | | ASP | 8 | 6.439 | 7.672 | 53.003 | 1.00 13.58 | ACPS |
| ATOM | 55 | C | ASP | 8 | 2.997 | 5.715 | 53.338 | 1.00 9.65 | ACPS |
| ATOM | 56 | 0 | ASP | 8 | 1.792 | 5.822 | 53.101 | 1.00 10.65 | ACPS |
| MOTA | 57 | N | ILE | 9 | 3.479 | 5.447 | 54.551 | 1.00 9.53 | ACPS |
| MOTA | 58 | CA | ILE | 9 | 2.598 | 5.334 | 55.721 | 1.00 9.56 | ACPS |
| ATOM | 59 | CB | ILE | 9 | 2.634 | 3.913 | 56.338 | 1.00 9.26 | ACPS |
| ATOM | 60 | | ILE | 9 | 1.780 | 3.890 | 57.602 | 1.00 10.57 | ACPS |
| ATOM | 61 | CG1 | | 9 | 2.101 | 2.881 | 55.338 | 1.00 9.47 | ACPS |
| ATOM | 62 | CD1 | | 9 | 2.215 | 1.426 | 55.815 | 1.00 10.23 | ACPS |
| ATOM | 63 | C | ILE | 9 | 3.142 | 6.361 | 56.717 | 1.00 9.80 | ACPS |
| MOTA | 64 | 0 | ILE | 9 | 4.233 | 6.206 | 57.245 | 1.00 9.76 | ACPS |
| ATOM | 65 | N | THR | 10 | 2.375 | 7.423 | 56.941 | 1.00 9.46 | ACPS |
| ATOM | 66 | CA | THR | 10 | 2.768 | 8.527 | 57.819 | 1.00 10.38 | ACPS |
| | | | | | | | | | |

| | ATOM | 67 | | | 10 | 2.428 | 9.871 | 57.089 | 1.00 10.26 | ACPS |
|-----|--------------|------------|---------|------------|------------|------------------|--------------------------|------------------|---------------------------------------|--------------|
| | ATOM | 68 | | | 10 | 3.340 | 10.050 | 55.997 | 1.00 11.15 | ACPS |
| | ATOM | 69 | | | 10 | 2.527 | 11.081 | 58.021 | 1.00 11.35 | ACPS |
| | ATOM | 70 | | THR | 10 | 2.113 | 8.453 | | 1.00 10.55 | ACPS |
| | MOTA | 71 | | THR | 10 | 0.936 | 8.111 | | 1.00 10.38 | ACPS |
| | ATOM | 72 | | GLU | 11 | 2.897 | 8.773 | 60.246 | 1.00 10.75 | ACPS |
| | ATOM | 73 | | | 11 | 2.463 | 8.743 | 61.654 | 1.00 11.46 | ACPS |
| | MOTA | 74 | | | 11 | 3.708 | 8.583 | 62.544 | 1.00 11.49 | ACPS |
| | MOTA | 75 | | | 11 | 3.454 | 8.435 | 64.044 | 1.00 14.01 | ACPS |
| | ATOM | 76 | | | 11 | 3.151 | 7.005 | | 1.00 16.01 | ACPS |
| | ATOM | 77 | | 1 GLU | 11 | 3.674 | 6.084 | | 1.00 17.38 | ACPS |
| | ATOM | 78 | | 2 GLU | 11 | 2.417 | 6.807 | 65.435 | 1.00 18.05 | ACPS |
| | ATOM | 79 | | GLU | 11 | 1.697 | 10.012 | 62.065 | 1.00 11.12 | ACPS |
| | ATOM | 80 | | GLU | 11 | 2.255 | 11.106 | 62.037 | 1.00 11.41 | ACPS |
| | ATOM ATOM | 81 82 | | LEU | 12 | 0.430 | 9.865 | 62.447 | 1.00 11.46 | ACPS |
| | ATOM | 83 | | | 12 | -0.383 | 11.026 | 62.848 | 1.00 12.27 | ACPS |
| | ATOM | 84 | | LEU | 12 | -1.785 | 10.582 | 63.305 | 1.00 12.68 | ACPS |
| | ATOM | 85 | | 1 LEU | 12 12 | -2.751 | 10.062 | 62.234 | 1.00 13.69 | ACPS |
| | MOTA | 86 | | 2 LEU | 12 | -4.049 -3.039 | 9.642 11. 1 40 | 62.918 | 1.00 13.86 | ACPS |
| | ATOM | 87 | | LEU | 12 | 0.265 | 11.140 | 61.183 63.963 | 1.00 14.80 | ACPS |
| | MOTA | 88 | ō | LEU | 12 | 0.270 | 13.066 | 63.915 | 1.00 1 2.67 1.00 1 2.56 | ACPS |
| | MOTA | 89 | N | LYS | 13 | 0.826 | 11.158 | 64.958 | 1.00 12.36 | ACPS |
| | MOTA | 90 | CA | LYS | 13 | 1.457 | 11.852 | 66.085 | 1.00 14.09 | ACPS |
| | MOTA | 91 | СВ | LYS | 13 | 1.878 | 10.851 | 67.165 | 1.00 15.99 | ACPS ACPS |
| A | MOTA | 92 | CG | LYS | 13 | 0.740 | 10.332 | 68.017 | 1.00 20.36 | ACPS |
| A | MOTA | 93 | CD | LYS | 13 | 1.290 | 9.557 | 69.197 | 1.00 23.47 | ACPS |
| A | MOTA | 94 | CE | LYS | 13 | 0.232 | 9.319 | 70.261 | 1.00 25.28 | ACPS |
| A | MOTA | 95 | NZ | LYS | 13 | 0.840 | 8.690 | 71.473 | 1.00 26.94 | ACPS |
| A | MOTA | 96 | C | LYS | 13 | 2.665 | 12.693 | 65.685 | 1.00 13.56 | ACPS |
| | MOTA | 97 | 0 | LYS | 13 | 2.924 | 13.738 | 66.295 | 1.00 13.25 | ACPS |
| | TOM | 98 | N | ARG | 14 | 3.423 | 12.237 | 64.692 | 1.00 12.75 | ACPS |
| | MOT | 99 | CA | ARG | 14 | 4.579 | 13.009 | 64.233 | 1.00 13.17 | ACPS |
| | MOT | 100 | CB | ARG | 14 | 5.436 | 12.178 | 63.270 | 1.00 14.59 | ACPS |
| | MOT | 101 | CG | ARG | 14 | 6.598 | 12.936 | 62.661 | 1.00 17.45 | ACPS |
| | TOM | 102 | CD | ARG | 14 | 7.572 | 12.010 | 61.933 | 1.00 21.04 | ACPS |
| | TOM | 103 | NE | ARG | 14 | 8.623 | 12.770 | 61.254 | 1.00 23.74 | ACPS |
| | TOM | 104 | CZ | ARG | 14 | 8.689 | 12.966 | 59.939 | 1.00 25.19 | ACPS |
| | TOM | 105 | | ARG | 14 | 7.768 | 12.450 | 59.134 | 1.00 25.79 | ACPS |
| | TOM TOM | 106 107 | | ARG | 14 | 9.671 | 13.701 | 59.425 | 1.00 25.80 | ACPS |
| | TOM | 108 | С 0 | ARG | 14 | 4.100 | 14.296 | 63.547 | 1.00 13.10 | ACPS |
| | TOM | 109 | _ | ARG | 14 | 4.636 | 15.377 | 63.798 | 1.00 13.21 | ACPS |
| | TOM | 110 | N CA | ILE ILE | 15 | 3.099 | 14.181 | 62.678 | 1.00 11.73 | ACPS |
| | TOM | 111 | СВ | ILE | 15 15 | 2.559 1.468 | 15.348 | 61.988 | 1.00 12.13 | ACPS |
| | TOM | 112 | | ILE | 15 | | 14.924 | 60.965 | 1.00 12.16 | ACPS |
| | TOM | 113 | | ILE | 15 | 0.822 | 16.150 | 60.320 | 1.00 13.81 | ACPS |
| | TOM | 114 | | ILE | 15 | 2.095 | 14.050 | 59.875 | 1.00 13.13 | ACPS |
| | TOM | 115 | C | ILE | 15 | 3.191 | 14.736 | 59.050 | 1.00 15.37 | ACPS |
| | TOM | 116 | 0 | ILE | 15 | 1.981 | 16.356 | 62.996 | 1.00 12.43 | ACPS |
| | TOM | 117 | N | ALA | 16 | 2.165 | 17.571 | 62.845 | 1.00 13.17 | ACPS |
| | TOM | 118 | CA | ALA | 16 | 1.292 0.711 | 15.859 | 64.019 | 1.00 12.31 | ACPS |
| | TOM | 119 | CB | ALA | 16 | | 16.740 | 65.038 | 1.00 13.48 | ACPS |
| | rom | 120 | C | ALA | 16 | -0.165 1.812 | 15.938 | 66.000 | 1.00 13.26 | ACPS |
| | FOM | 121 | 0 | ALA | 16 | 1.679 | 17.456 | 65.811 | 1.00 13.84 | ACPS |
| | MOT | 122 | N | SER | 17 | 2.902 | 18.631 | 66.159 | 1.00 14.13 | ACPS |
| | MOT | 123 | CA | SER | 17 | 4.013 | 16.752 | 66.089 | 1.00 13.89 | ACPS |
| *** | | *** | | 221 | - ' | 4.013 | 17.356 | 66.809 | 1.00 14.78 | ACPS |
| | | | | | | | | | | |

| MOTA | 124 | CB | SER | 17 | 5.041 | 16.291 | 67.199 | 1.00 14.52 | ACPS |
|------|-----|-----|-----|----|--------|----------------|--------|------------|------|
| ATOM | 125 | | SER | 17 | 6.151 | 16.878 | 67.861 | 1.00 15.33 | ACPS |
| ATOM | 126 | C | SER | 17 | 4.686 | 18.440 | 65.971 | 1.00 15.57 | ACPS |
| MOTA | 127 | 0 | SER | 17 | 4.981 | 19.528 | 66.478 | 1.00 16.23 | ACPS |
| MOTA | 128 | N | MET | 18 | 4.933 | 18.163 | 64.694 | 1.00 15.86 | ACPS |
| MOTA | 129 | CA | MET | 18 | 5.568 | 19.173 | 63.861 | 1.00 17.36 | ACPS |
| ATOM | 130 | CB | MET | 18 | 5.920 | 18.593 | 62.491 | 1.00 18.79 | ACPS |
| ATOM | 131 | CG | MET | 18 | 6.984 | 17.513 | 62.579 | 1.00 21.58 | ACPS |
| ATOM | 132 | SD | MET | 18 | 7.569 | 16.962 | 60.979 | 1.00 27.23 | ACPS |
| ATOM | 133 | CE | MET | 18 | 6.322 | 15.823 | 60.550 | 1.00 24.77 | ACPS |
| ATOM | 134 | C | MET | 18 | 4.679 | 20.408 | 63.724 | 1.00 18.05 | ACPS |
| MOTA | 135 | 0 | MET | 18 | 5.171 | 21.537 | 63.720 | 1.00 17.78 | ACPS |
| ATOM | 136 | N | ALA | 19 | 3.371 | 20.200 | 63.637 | 1.00 17.79 | ACPS |
| MOTA | 137 | CA | ALA | 19 | 2.439 | 21.320 | 63.519 | 1.00 19.33 | ACPS |
| ATOM | 138 | CB | ALA | 19 | 1.047 | 20.810 | 63.161 | 1.00 18.47 | ACPS |
| MOTA | 139 | С | ALA | 19 | 2.391 | 22.119 | 64.827 | 1.00 20.49 | ACPS |
| MOTA | 140 | 0 | ALA | 19 | 2.124 | 23.324 | 64.820 | 1.00 21.87 | ACPS |
| ATOM | 141 | N | GLY | 20 | 2.655 | 21.446 | 65.944 | 1.00 21.04 | ACPS |
| ATOM | 142 | CA | GLY | 20 | 2.635 | 22.112 | 67.234 | 1.00 22.79 | ACPS |
| MOTA | 143 | С | GLY | 20 | 3.916 | 22.879 | 67.506 | 1.00 24.03 | ACPS |
| ATOM | 144 | 0 | GLY | 20 | 3.920 | 23.834 | 68.283 | 1.00 25.21 | ACPS |
| ATOM | 145 | N | ARG | 21 | 5.007 | 22.463 | 66.875 | 1.00 24.92 | ACPS |
| ATOM | 146 | CA | ARG | 21 | 6.286 | 23.135 | 67.062 | 1.00 26.49 | ACPS |
| ATOM | 147 | CB | ARG | 21 | 7.420 | 22.117 | 67.058 | 1.00 27.00 | ACPS |
| ATOM | 148 | CG | ARG | 21 | 7.376 | 21.144 | 68.216 | 1.00 28.19 | ACPS |
| MOTA | 149 | CD | ARG | 21 | 8.764 | 20.607 | 68.471 | 1.00 29.42 | ACPS |
| MOTA | 150 | NE | ARG | 21 | 9.667 | 21.695 | 68.835 | 1.00 30.12 | ACPS |
| MOTA | 151 | CZ | ARG | 21 | 10.993 | 21.603 | 68.834 | 1.00 29.99 | ACPS |
| ATOM | 152 | NH1 | ARG | 21 | 11.727 | 22.650 | 69.183 | 1.00 30.82 | ACPS |
| ATOM | 153 | NH2 | ARG | 21 | 11.584 | 20.469 | 68.481 | 1.00 30.49 | ACPS |
| MOTA | 154 | C | ARG | 21 | 6.559 | 24.208 | 66.006 | 1.00 27.49 | ACPS |
| MOTA | 155 | 0 | ARG | 21 | 7.329 | 25.141 | 66.247 | 1.00 28.27 | ACPS |
| MOTA | 156 | N | GLN | 22 | 5.935 | 24.073 | 64.840 | 1.00 27.79 | ACPS |
| MOTA | 157 | CA | GLN | 22 | 6.103 | 25.039 | 63.757 | 1.00 28.18 | ACPS |
| MOTA | 158 | CB | GLN | 22 | 6.697 | 24.364 | 62.515 | 1.00 29.33 | ACPS |
| MOTA | 159 | CG | GLN | 22 | 8.186 | 24.075 | 62.625 | 1.00 30.67 | ACPS |
| ATOM | 160 | CD | GLN | 22 | 8.839 | 23.775 | 61.284 | 1.00 31.99 | ACPS |
| ATOM | 161 | | GLN | 22 | 10.065 | 23.853 | 61.148 | 1.00 33.50 | ACPS |
| ATOM | 162 | | GLN | 22 | 8.029 | 23.422 | 60.291 | 1.00 31.08 | ACPS |
| MOTA | 163 | | GLN | 22 | 4.765 | 25.6 86 | 63.406 | 1.00 27.71 | ACPS |
| MOTA | 164 | 0 | GLN | 22 | 3.866 | 25.036 | 62.869 | 1.00 27.85 | ACPS |
| ATOM | 165 | N | ALA | 23 | 4.646 | | | 1.00 26.91 | ACPS |
| ATOM | 166 | CA | ALA | 23 | 3.420 | 27.721 | 63.453 | 1.00 25.59 | ACPS |
| ATOM | 167 | CB | ALA | 23 | 3.578 | 29.155 | 63.945 | 1.00 26.37 | ACPS |
| MOTA | 168 | C | ALA | 23 | 2.966 | 27.722 | 61.994 | 1.00 24.20 | ACPS |
| ATOM | 169 | 0 | ALA | 23 | 1.784 | 27.936 | 61.711 | 1.00 25.27 | ACPS |
| ATOM | 170 | N | ARG | 24 | 3.885 | 27.478 | 61.068 | 1.00 22.39 | ACPS |
| ATOM | 171 | CA | ARG | 24 | 3.519 | 27.481 | 59.655 | 1.00 20.64 | ACPS |
| MOTA | 172 | CB | ARG | 24 | 4.265 | 28.617 | 58.943 | 1.00 23.30 | ACPS |
| MOTA | 173 | CG | ARG | 24 | 4.063 | 29.987 | 59.612 | 1.00 26.19 | ACPS |
| MOTA | 174 | CD | ARG | 24 | 4.793 | 31.085 | 58.862 | 1.00 30.07 | ACPS |
| ATOM | 175 | NE | ARG | 24 | 4.710 | 32.403 | 59.493 | 1.00 32.13 | ACPS |
| MOTA | 176 | CZ | ARG | 24 | 5.594 | 32.879 | 60.363 | 1.00 32.86 | ACPS |
| MOTA | 177 | NH1 | | 24 | 6.644 | 32.150 | 60.720 | 1.00 33.10 | ACPS |
| MOTA | 178 | NH2 | ARG | 24 | 5.435 | 34.097 | 60.867 | 1.00 34.22 | ACPS |
| MOTA | 179 | C | ARG | 24 | 3.784 | 26.144 | 58.956 | 1.00 19.11 | ACPS |
| ATOM | 180 | 0 | ARG | 24 | 3.982 | 26.094 | 57.744 | 1.00 17.80 | ACPS |
| | | | | | | | | | |

| | | | | - | | | | | |
|--------------|------------|----------|------------|----------|------------------|------------------|------------------|--------------------------|------|
| ATOM | 18: | | PHE | 25 | 3.765 | | 59.720 | 1.00 16.89 | ACPS |
| ATOM | 182 | | | 25 | 4.007 | | | 1.00 16.15 | ACPS |
| ATOM | 183 | | | 25 | 3.958 | | 60.246 | 1.00 16.22 | ACPS |
| MOTA | 184 | • | | 25 | 4.308 | 21.282 | 59.757 | 1.00 16.81 | ACPS |
| MOTA | 185 | | 1 PHE | 25 | 3.357 | 20.271 | . 59. 754 | 1.00 17.39 | ACPS |
| ATOM | 186 | | 2 PHE | 25 | 5.57 7 | | | 1.00 16.97 | ACPS |
| ATOM | 187 | | 1 PHE | 25 | 3.662 | . 19.001 | 59.253 | 1.00 18.39 | ACPS |
| ATOM | 188 | | | 25 | 5.892 | 19.737 | 58.752 | | ACPS |
| ATOM | 189 | | | 25 | 4.930 | 18.737 | 58.753 | | ACPS |
| MOTA | 190 | | PHE | 25 | 3.038 | 23.370 | 58.015 | | ACPS |
| MOTA | 191 | | PHE | 25 | 3.464 | 22.840 | 56.988 | 1.00 14.64 | ACPS |
| ATOM | 192 | | ALA | 26 | 1.748 | 23.646 | 5 8. 196 | | ACPS |
| MOTA | 193 | | | 26 | 0.762 | 23.332 | | | ACPS |
| ATOM | 194 | | | 26 | -0.658 | 23.670 | 57.642 | 1.00 16.24 | ACPS |
| ATOM | 195 | | ALA | 26 | 1.075 | 24.093 | 55.881 | 1.00 15.52 | ACPS |
| ATOM | 196 | | ALA | 26 | 0.941 | 23.551 | 54.787 | 1.00 14.18 | ACPS |
| ATOM | 197 | | GLU | 27 | 1.512 | 25.345 | 56.011 | 1.00 14.73 | ACPS |
| ATOM | 198 | | | 27 | 1.839 | 26.155 | 54.838 | 1.00 15.35 | ACPS |
| MOTA | 199 | | GLU | 27 | 2.041 | 27.619 | 5 5.2 36 | 1.00 16.37 | ACPS |
| ATOM | 200 | | | 27 | 0.782 | 28.381 | 55.603 | 1.00 18.60 | ACPS |
| ATOM | 201 | | GLU | 27 | 0.176 | 27.956 | 56.927 | 1.00 19.31 | ACPS |
| MOTA | 202 | | 1 GLU | 27 | 0.899 | 27.430 | 5 7. 796 | 1.00 19.16 | ACPS |
| ATOM | 203 | OE: | | 27 | -1.040 | 28.169 | 5 7 .109 | 1.00 22.95 | ACPS |
| ATOM | 204 | C | GLU | 27 | 3.089 | 25.652 | 54.115 | 1.00 14.38 | ACPS |
| ATOM | 205 | 0 | GLU | 27 | 3.309 | 25.946 | 52.944 | 1.00 14.80 | ACPS |
| ATOM | 206 | N | ARG | 28 | 3.907 | 24.896 | 54.829 | 1.00 15.20 | ACPS |
| ATOM | 207 | CA | ARG | 28 | 5.119 | 24.330 | 54.268 | 1.00 16.00 | ACPS |
| ATOM | 208 | CB | ARG | 28 | 6.018 | 23.880 | 55.420 | 1.00 18.75 | ACPS |
| ATOM ATOM | 209 210 | CG | ARG | 28 | 7.335 | 23.289 | 55.015 | 1.00 22.72 | ACPS |
| ATOM | 210 | CD NE | ARG | 28 | 8.158 | 22.968 | 56.250 | 1.00 25.44 | ACPS |
| ATOM | 211 | CZ | ARG ARG | 28 | 9.461 | | 55.890 | 1.00 28.04 | ACPS |
| ATOM | 213 | | ARG ARG | 28 | 10.382 | 22.070 | 56.775 | 1.00 28.40 | ACPS |
| ATOM | 214 | NH2 | | 28 28 | 11.542 | 21.594 | 56.356 | 1.00 29.55 | ACPS |
| ATOM | 215 | C | ARG | 28 | 10.135 | 22.184 | 58.074 | 1.00 28.44 | ACPS |
| ATOM | 216 | o | ARG | 28 | 4.768 5.345 | 23.129 | 53.380 | 1.00 15.03 | ACPS |
| ATOM | 217 | N | ILE | 29 | 3.792 | 22.925 22.350 | 52.311 | 1.00 15.61 | ACPS |
| ATOM | 218 | CA | ILE | 29 | 3.792 | 21.137 | 53.824 | 1.00 14.41 | ACPS |
| ATOM | 219 | CB | ILE | 29 | 2.883 | 20.066 | 53.112 | 1.00 14.00 | ACPS |
| ATOM | 220 | | ILE | 29 | 2.586 | 18.765 | 54 - 121 | 1.00 13.17 | ACPS |
| ATOM | 221 | | ILE | 29 | 3.900 | 19.834 | 53.401 55.245 | 1.00 13.59 | ACPS |
| ATOM | 222 | | ILE | 29 | 5.307 | | _ | 1.00 13.14 | ACPS |
| ATOM | 223 | C | ILE | 29 | 2.313 | 19.516 21.299 | 54.785 52.034 | 1.00 12.95 1.00 13.32 | ACPS |
| ATOM | 224 | ō | ILE | 29 | 2.370 | 20.650 | 50_993 | | ACPS |
| ATOM | 225 | N | LEU | 30 | 1.350 | 20.650 | | 1.00 13.97 | ACPS |
| ATOM | 226 | CA | LEU | 30 | 0.211 | 22.337 | 52.275 | 1.00 12.58 | ACPS |
| ATOM | 227 | CB | LEU | 30 | -1.073 | 22.337 | 51.369 | 1.00 12.60 | ACPS |
| ATOM | 228 | CG | LEU | 30 | -1.309 | 21.263 | 52_207 | 1.00 12.43 | ACPS |
| ATOM | 229 | | LEU | 30 | -2.536 | | 53.220 | 1.00 12.14 | ACPS |
| ATOM | 230 | | LEU | 30 | -2.336 | 21.595 | 54_057 | 1.00 13.80 | ACPS |
| ATOM | 231 | C | LEU | 30 | 0.227 | 19.932 | 52.491 | 1.00 12.77 | ACPS |
| ATOM | 232 | ō | LEU | 30 | 0.227 | 23.540 | 50.432 | 1.00 12.66 | ACPS |
| ATOM | 233 | N | THR | 31 | | 24.605 | 50.785 | 1.00 14.05 | ACPS |
| ATOM | 234 | CA | THR | 31 | -0.342 -0.456 | 23.359 | 49_242 | 1.00 13.04 | ACPS |
| ATOM | 235 | CB | THR | 31 | -0.456 | 24.450 | 48.265 | 1.00 13.14 | ACPS |
| ATOM | 236 | | THR | 31 | -0.746 | 23.921 | 46.859 | 1.00 13.54 | ACPS |
| ATOM | 237 | CG2 | | 31 | -2.018 | 23.262 | 46 - 854 | 1.00 13.92 | ACPS |
| | | - | **** | J. | 0.313 | 22.937 | 46-429 | 1.00 14.69 | ACPS |
| | | | | | | | | | |

| MOTA | 238 | | THR | 31 | -1.641 | 25.32 8 | 48.690 | 1.00 13.91 | ACPS |
|--------------|------------|----------|------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 239 | | THR | 31 | -2.374 | 24.980 | 49.617 | 1.00 13.14 | ACPS |
| ATOM | 240 | N | ARG | 32 | -1.836 | 26.45 5 | 48.014 | 1.00 15.34 | ACPS |
| MOTA | 241 | | | 32 | -2.947 | 27.338 | 48.367 | 1.00 15.55 | ACPS |
| MOTA | 242 | | | 32 | -2.912 | 28.61 5 | 47.517 | 1.00 16.36 | ACPS |
| ATOM | 243 | ÇG | ARG | 32 | -1.630 | 29.403 | 47.682 | 1.00 18.69 | ACPS |
| ATOM | 244 | CD | ARG | 32 | -1.794 | 30.834 | 47.191 | 1.00 20.77 | ACPS |
| MOTA | 245 | NE | ARG | 32 | -2.750 | 31.590 | 48.000 | 1.00 22.37 | ACPS |
| ATOM | 246 | | - | 32 | -3.938 | 32.003 | 47.569 | 1.00 23.12 | ACPS |
| ATOM | 247 | NH | 1 ARG | 32 | -4.326 | 31.738 | 46.330 | 1.00 23.58 | ACPS |
| MOTA | 248 | NH: | 2 ARG | 32 | -4.738 | 32.686 | 48.380 | 1.00 22.27 | ACPS |
| ATOM | 249 | C | ARG | 32 | -4.296 | 26.646 | 48.205 | 1.00 15.92 | ACPS |
| ATOM | 250 | 0 | ARG | 32 | -5.166 | 26.781 | 49.054 | 1.00 16.02 | ACPS |
| ATOM | 251 | N | SER | 33 | -4.467 | 25.908 | 47.114 | 1.00 16.47 | ACPS |
| ATOM | 252 | CA | SER | 33 | -5.717 | 25.183 | 46.863 | 1.00 16.46 | ACPS |
| ATOM | 253 | CB | SER | 33 | -5.638 | 24.465 | 45.513 | 1.00 17.75 | ACPS |
| ATOM | 254 | OG | SER | 33 | -6.833 | 23.772 | 45.224 | 1.00 24.08 | ACPS |
| ATOM | 255 | C | SER | 33 | -5.981 | 24.154 | 47.967 | 1.00 16.53 | ACPS |
| ATOM | 256 | 0 | SER | 33 | -7.115 | 23.963 | 48.404 | 1.00 16.86 | ACPS |
| MOTA | 257 | N | GLU | 34 | -4.926 | 23.484 | 48.413 | 1.00 15.70 | ACPS |
| MOTA | 258 | CA | GLU | 34 | -5.058 | 22.480 | 49.458 | 1.00 15.77 | ACPS |
| ATOM | 259 | CB | GLU | 34 | -3.753 | 21.67 7 | 49.573 | 1.00 14.72 | ACPS |
| ATOM | 260 | CG | GLU | 34 | -3.578 | 20.659 | 48.459 | 1.00 15.35 | ACPS |
| MOTA | 261 | CD | GLU | 34 | -2.174 | 20.079 | 48.369 | 1.00 13.75 | ACPS |
| MOTA | 262 | | GLU | 34 | -2.023 | 19.029 | 47.719 | 1.00 13.81 | ACPS |
| ATOM | 263 | OE2 | | 34 | -1.215 | 20.669 | 48.916 | 1.00 13.16 | ACPS |
| ATOM | 264 | C | GLU | 34 | -5.397 | 23.134 | 50.789 | 1.00 15.99 | ACPS |
| ATOM | 265 | 0 | GLU | 34 | -6.206 | 22.621 | 51.563 | 1.00 17.16 | ACPS |
| MOTA | 266 | N | LEU | 35 | -4.781 | 24.285 | 51.050 | 1.00 16.62 | ACPS |
| ATOM | 267 | CA | LEU | 35 | -5.025 | 25.008 | 52.285 | 1.00 17.38 | ACPS |
| ATOM | 268 | CB CG | LEU | 35 | -4.064 | 26.199 | 52.401 | 1.00 17.16 | ACPS |
| MOTA MOTA | 269 270 | | LEU LEU | 35 35 | -2.614 | 25.863 | 52.761 | 1.00 17.73 | ACPS |
| ATOM | 271 | | LEU | 35 | -1.722 -2.547 | 27.078 | 52.532 | 1.00 17.25 | ACPS |
| ATOM | 272 | C | LEU | . 35 | -6.462 | 25.405 25.499 | 54.212 | 1.00 17.05 | ACPS |
| ATOM | 273 | o | LEU | 35 | -7.035 | 25.535 | 52.380 53.466 | 1.00 18.36 1.00 17.94 | ACPS |
| ATOM | 274 | Ŋ | ASP | 36 | -7.049 | 25.866 | 51.248 | 1.00 17.34 | ACPS |
| ATOM | 275 | CA | ASP | 36 | -8.419 | 26.361 | 51.264 | 1.00 19.36 | ACPS |
| ATOM | 276 | CB | ASP | 36 | -8.866 | 26.738 | 49.845 | 1.00 22.68 | ACPS ACPS |
| ATOM | 277 | CG | ASP | 36 | -9.949 | 27.806 | 49.836 | 1.00 24.19 | ACPS |
| ATOM | 278 | | ASP | 36 | -9.928 | 28.690 | 50.724 | 1.00 25.68 | ACPS |
| ATOM | 279 | | ASP | 36 | -10.807 | 27.773 | | 1.00 24.47 | ACPS |
| ATOM | 280 | C | ASP | 36 | -9.321 | 25.285 | 51.857 | 1.00 22.68 | ACPS |
| ATOM | 281 | 0 | ASP | 36 | -10.269 | 25.589 | 52.587 | 1.00 23.58 | ACPS |
| ATOM | 282 | N | GLN | 37 | -9.003 | 24.024 | 51.572 | 1.00 22.62 | ACPS |
| ATOM | 283 | CA | GLN | 37 | -9.784 | 22.899 | 52.087 | 1.00 23.62 | ACPS |
| ATOM | 284 | СВ | GLN | 37 | -9.514 | 21.653 | 51.236 | 1.00 24.76 | ACPS |
| ATOM | 285 | CG | GLN | 37 | -9.899 | 21.812 | 49.769 | 1.00 26.90 | ACPS |
| MOTA | 286 | CD | GLN | 37 | -9.264 | 20.761 | 48.867 | 1.00 29.15 | ACPS |
| ATOM | 287 | | GLN | 37 | -9.409 | 19.557 | 49.092 | 1.00 30.76 | ACPS |
| ATOM | 288 | | GLN | 37 | -8.556 | 21.215 | 47.836 | 1.00 30.60 | ACPS |
| ATOM | 289 | C | GLN | 37 | -9.445 | 22.617 | 53.554 | 1.00 23.33 | ACPS |
| ATOM | 290 | ō | GLN | 37 | -10.321 | 22.331 | 54.367 | 1.00 23.33 | ACPS |
| ATOM | 291 | N | TYR | 38 | -8.161 | 22.711 | 53.876 | 1.00 23.30 | ACPS |
| ATOM | 292 | CA | TYR | 38 | -7.644 | 22.474 | 55.222 | 1.00 22.41 | ACPS |
| ATOM | 293 | CB | TYR | 38 | -6.115 | 22.564 | 55.169 | 1.00 22.14 | ACPS |
| ATOM | 294 | CG | TYR | 38 | -5.376 | 22.533 | 56.491 | 1.00 20.71 | ACPS |
| | | | | | 3.370 | -L.JJJ | 20.421 | 1.00 20.71 | ACPS |

| MOTA | 295 | | 1 TYR | 38 | -4.945 | 23.711 | | | ACPS |
|------|-----|-----|-------|----------|---------|--------|--------|--------------------------|------|
| MOTA | 296 | CE: | 1 TYR | 38 | -4.180 | 23.677 | 58.276 | 1.00 21.07 | ACPS |
| MOTA | 297 | CD: | 2 TYR | 38 | -5.033 | 21.322 | 57.084 | 1.00 19.25 | ACPS |
| MOTA | 298 | CE: | 2 TYR | 38 | -4.275 | 21.276 | 58.246 | 1.00 20.56 | ACPS |
| ATOM | 299 | CZ | TYR | 38 | ~3.848 | 22.451 | 58.837 | 1.00 21.15 | ACPS |
| ATOM | 300 | OH | TYR | 38 | -3.079 | 22.392 | 59.976 | 1.00 21.86 | ACPS |
| MOTA | 301 | С | TYR | 38 | -8.191 | 23.441 | 56.270 | 1.00 22.57 | ACPS |
| ATOM | 302 | | TYR | 38 | -8.599 | 23.031 | 57.357 | 1.00 21.64 | ACPS |
| ATOM | 303 | N | TYR | 39 | -8.201 | 24.727 | 55.933 | 1.00 23.00 | ACPS |
| ATOM | 304 | | TYR | 39 | -8.669 | 25.750 | 56.854 | 1.00 23.93 | ACPS |
| ATOM | 305 | СВ | TYR | 39 | -8.540 | 27.139 | 56.212 | 1.00 24.42 | ACPS |
| ATOM | 306 | CG | TYR | 39 | -7.117 | 27.588 | 55.948 | 1.00 25.39 | ACPS |
| ATOM | 307 | | LTYR | 39 | -6.061 | 27.134 | 56.734 | 1.00 26.23 | ACPS |
| ATOM | 308 | CEI | | 39 | -4.763 | 27.590 | 56.525 | 1.00 20.23 | ACPS |
| ATOM | 309 | CD2 | | 39 | -6.836 | 28.512 | 54.939 | 1.00 27.43 | |
| ATOM | 310 | CE2 | | 39. | -5.540 | 28.979 | 54.726 | 1.00 26.81 | ACPS |
| ATOM | 311 | CZ | TYR | 39 | -4.508 | 28.516 | 55.522 | | ACPS |
| ATOM | 312 | OH | TYR | 39 | -3.224 | 28.999 | 55.322 | 1.00 27.95 1.00 28.86 | ACPS |
| ATOM | 313 | C | TYR | 39 | -10.095 | 25.568 | | | ACPS |
| ATOM | 314 | | | | | | 57.369 | 1.00 24.48 | ACPS |
| | | 0 | TYR | 39 40 | -10.440 | 26.118 | 58.412 | 1.00 25.01 | ACPS |
| ATOM | 315 | N | GLU | 40 | -10.916 | 24.802 | 56.656 | 1.00 24.88 | ACPS |
| ATOM | 316 | CA | GLU | 40 | -12.307 | 24.591 | 57.067 | 1.00 26.05 | ACPS |
| ATOM | 317 | CB | GLU | 40 | -13.180 | 24.249 | 55.854 | 1.00 27.82 | ACPS |
| ATOM | 318 | CG | GLU | 40 | -13.036 | 25.174 | 54.661 | 1.00 30.61 | ACPS |
| ATOM | 319 | CD | GLU | 40 | -14.017 | 24.833 | 53.551 | 1.00 31.77 | ACPS |
| ATOM | 320 | OE1 | | 40 | -14.101 | 23.640 | 53.178 | 1.00 32.73 | ACPS |
| ATOM | 321 | OE2 | | 40 | -14.697 | 25.756 | 53.050 | 1.00 33.34 | ACPS |
| ATOM | 322 | C | GLU | 40 | -12.487 | 23.467 | 58.086 | 1.00 25.59 | ACPS |
| ATOM | 323 | 0 | GLU | 40 | -13.581 | 23.280 | 58.618 | 1.00 26.05 | ACPS |
| ATOM | 324 | N | LEU | 41 | -11.420 | 22.731 | 58.368 | 1.00 24.07 | ACPS |
| ATOM | 325 | CA | LEU | 41 | -11.509 | 21.584 | 59.266 | 1.00 22.24 | ACPS |
| ATOM | 326 | CB | LEU | 41 | -10.578 | 20.486 | 58.744 | 1.00 21.78 | ACPS |
| ATOM | 327 | CG | LEU | 41 | -10.760 | 20.090 | 57.273 | 1.00 21.91 | ACPS |
| ATOM | 328 | | LEU | 41 | -9.666 | 19.107 | 56.881 | 1.00 21.70 | ACPS |
| ATOM | 329 | | LEU | 41 | -12.126 | 19.474 | 57.058 | 1.00 22.12 | ACPS |
| ATOM | 330 | C | LEU | 41 | -11.230 | 21.813 | 60.748 | 1.00 21.46 | ACPS |
| MOTA | 331 | 0 | LEU | 41 | -10.614 | 22.800 | 61.141 | 1.00 21.25 | ACPS |
| ATOM | 332 | N | SER | 42 | -11.693 | 20.873 | 61.567 | 1.00 21.01 | ACPS |
| ATOM | 333 | CA | SER | 42 | -11.476 | 20.926 | 63.009 | 1.00 20.67 | ACPS |
| ATOM | 334 | CB | SER | 42 | -12.319 | 19.865 | 63.716 | 1.00 21.24 | ACPS |
| MOTA | 335 | OG | SER | 42 | -11.874 | 18.558 | 63.388 | 1.00 20.80 | ACPS |
| MOTA | 336 | С | SER | 42 | -10.008 | 20.617 | 63.245 | 1.00 20.69 | ACPS |
| MOTA | 337 | 0 | SER | 42 | -9.309 | 20.184 | 62.328 | 1.00 19.86 | ACPS |
| ATOM | 338 | N | GLU | 43 | -9.540 | 20.834 | 64.469 | 1.00 19.62 | ACPS |
| ATOM | 339 | CA | GLU | 43 | -8.146 | 20.568 | 64.815 | 1.00 19.23 | ACPS |
| ATOM | 340 | CB | GLU | 43 | -7.932 | 20.830 | 66.312 | 1.00 20.39 | ACPS |
| ATOM | 341 | CG | GLU | 43 | -6.524 | 20.541 | 66.843 | 1.00 22.14 | ACPS |
| ATOM | 342 | CD | GLU | 43 | -6.452 | 20.617 | 68.366 | 1.00 23.47 | ACPS |
| ATOM | 343 | OE1 | GLU | 43 | -6.731 | 21.698 | 68.922 | 1.00 23.93 | ACPS |
| ATOM | 344 | | GLU | 43 | -6.118 | 19.594 | 69.004 | 1.00 24.66 | ACPS |
| ATOM | 345 | С | GLU | 43 | -7.789 | 19.120 | 64.473 | 1.00 18.65 | ACPS |
| ATOM | 346 | ō | GLU | 43 | -6.755 | 18.849 | 63.864 | 1.00 18.62 | ACPS |
| ATOM | 347 | N | LYS | 44 | -8.653 | 18.190 | 64.853 | 1.00 17.32 | ACPS |
| ATOM | 348 | CA | LYS | 44 | -8.403 | 16.777 | 64.591 | 1.00 17.32 | ACPS |
| ATOM | 349 | CB | LYS | 44 | | | | | |
| | | CG | LYS | | -9.441 | 15.931 | 65.326 | 1.00 16.54 | ACPS |
| ATOM | 350 | | | 44 | -9.404 | 14.452 | 64.984 | 1.00 17.99 | ACPS |
| ATOM | 351 | CD | LYS | 44 | -10.561 | 13.732 | 65.664 | 1.00 19.56 | ACPS |
| | | | | | | | | | |

| MOTA | 352 | | LYS | 44 | -10.691 | 12.285 | | 1.00 19.17 | ACPS |
|------|-----|------|-------|------|---------|-----------------|--------------------|------------|------|
| ATOM | 353 | | LYS | 44 | -11.159 | 12.153 | 63.799 | 1.00 19.63 | ACPS |
| ATOM | 354 | С | LYS | 44 | -8.413 | 16.431 | 63.099 | 1.00 16.56 | ACPS |
| ATOM | 355 | 0 | LYS | 44 | -7.530 | 15.719 | 62.613 | 1.00 16.25 | ACPS |
| ATOM | 356 | N | ARG | 45 | -9.412 | 16.923 | 62.375 | 1.00 16.89 | ACPS |
| ATOM | 357 | CA | ARG | 45 | -9.507 | 16.641 | 60.947 | 1.00 17.08 | ACPS |
| ATOM | 358 | CB | ARG | 45 | -10.849 | 17.131 | 60.400 | 1.00 19.32 | ACPS |
| MOTA | 359 | CG | ARG | 45 | -12.053 | 16.345 | 60.910 | 1.00 21.73 | ACPS |
| ATOM | 360 | CD | ARG | 45 | -12.092 | 14.927 | 60.336 | 1.00 25.16 | ACPS |
| ATOM | 361 | NE | ARG | 45 | -13.304 | 14.213 | 60.741 | 1.00 28.95 | ACPS |
| ATOM | 362 | CZ | ARG | 45 | -13.616 | 12.977 | 60.360 | 1.00 30.49 | ACPS |
| MOTA | 363 | NHI | L ARG | 45 | -14.743 | 12.419 | 60.783 | 1.00 31.89 | ACPS |
| MOTA | 364 | NH2 | 2 ARG | 45 | -12.808 | 12.296 | 59.553 | 1.00 32.45 | ACPS |
| ATOM | 365 | C | ARG | 45 | -8.353 | 17.284 | 60.189 | 1.00 16.29 | ACPS |
| MOTA | 366 | 0 | ARG | 45 | -7.871 | 16.734 | 59.198 | 1.00 15.72 | ACPS |
| MOTA | 367 | N | LYS | 46 | -7.917 | 18.455 | 60.644 | 1.00 15.52 | ACPS |
| ATOM | 368 | CA | LYS | 46 | -6.796 | 19.128 | 60.009 | 1.00 15.32 | ACPS |
| ATOM | 369 | CB | LYS | 46 | -6.449 | 20.429 | 60.746 | 1.00 15.53 | ACPS |
| ATOM | 370 | CG | LYS | 46 | -7.232 | 21.666 | 60.320 | 1.00 18.65 | ACPS |
| MOTA | 371 | CD | LYS | 46 | -6.678 | 22.887 | 61.051 | 1.00 20.77 | ACPS |
| ATOM | 372 | CE | LYS | 46 | -7.201 | 24.203 | 60.485 | 1.00 22.56 | ACPS |
| ATOM | 373 | NZ | LYS | 46 | -8.661 | 24.396 | 60.688 | 1.00 24.62 | ACPS |
| MOTA | 374 | С | LYS | 46 | -5.584 | 18.207 | 60.036 | 1.00 14.61 | ACPS |
| MOTA | 375 | 0 | LYS | 46 | -4.892 | 18.051 | 59.033 | 1.00 14.78 | ACPS |
| MOTA | 376 | N | ASN | 47 | -5.320 | 17.602 | 61.190 | 1.00 14.97 | ACPS |
| ATOM | 377 | CA | ASN | 47 | -4.174 | 16.711 | 61.329 | 1.00 14.85 | ACPS |
| MOTA | 378 | CB | ASN | 47 | -4.064 | 16.233 | 62.783 | 1.00 16.85 | ACPS |
| MOTA | 379 | CG | ASN | 47 | -2.877 | 15.317 | 63.008 | 1.00 19.82 | ACPS |
| MOTA | 380 | OD1 | ASN | 47 | -1.732 | 15.704 | 62.794 | 1.00 22.35 | ACPS |
| MOTA | 381 | ND2 | ASN | 47 | -3.149 | 14.093 | `63.439 | 1.00 21.62 | ACPS |
| MOTA | 382 | G· , | ASN | 47 | -4.283 | 15.517 | 60.373 | 1.00 14.22 | ACPS |
| MOTA | 383 | 0 | ASN | 47 | -3.312 | 15.159 | 59.702 | 1.00 13.37 | ACPS |
| MOTA | 384 | N | GLU | 48 | -5.461 | 14.915 | 60.289 | 1.00 13.02 | ACPS |
| MOTA | 385 | CA | GLU | 48 | -5.650 | 13.774 | 59.392 | 1.00 13.33 | ACPS |
| MOTA | 386 | CB | GLU | 48 | -7.005 | 13.122 | 59.66 6 | 1.00 13.97 | ACPS |
| MOTA | 387 | CG | GLU | 48 | -7.094 | 12.540 | 61.075 | 1.00 17.87 | ACPS |
| MOTA | 388 | CD | GLU | 48 | -8.518 | 12.306 | 61.525 | 1.00 19.35 | ACPS |
| MOTA | 389 | | GLU | 48 | -8.699 | 11.814 | 62.65 7 | 1.00 22.50 | ACPS |
| MOTA | 390 | | GLU | 48 | -9.449 | 12.615 | 60.754 | 1.00 22.51 | ACPS |
| ATOM | 391 | C | GLU | 48 | -5.531 | 14.180 | 57.925 | 1.00 12.99 | ACPS |
| ATOM | 392 | 0 | GLU | 48 | -4.927 | 13.463 | 57.121 | 1.00 12.41 | ACPS |
| ATOM | 393 | N | PHE | 49 | -6.098 | 15.331 | 57.573 | 1.00 12.16 | ACPS |
| ATOM | 394 | CA | PHE | 49 | -6.015 | 15.818 | 56.204 | 1.00 11.74 | ACPS |
| MOTA | 395 | CB | PHE | . 49 | -6.827 | 17.118 | 56.058 | 1.00 12.28 | ACPS |
| MOTA | 396 | CG | PHE | 49 | -6.785 | 17.716 | 54.674 | 1.00 13.38 | ACPS |
| MOTA | 397 | | PHE | 49 | -7.742 | 1 7 .379 | 53.724 | 1.00 13.30 | ACPS |
| MOTA | 398 | CD2 | PHE | 49 | -5.794 | 18.626 | 54.324 | 1.00 12.58 | ACPS |
| MOTA | 399 | | PHE | 49 | -7.710 | 17.950 | 52.449 | 1.00 14.47 | ACPS |
| MOTA | 400 | CE2 | PHE | 49 | -5.754 | 19.197 | 53.058 | 1.00 13.76 | ACPS |
| MOTA | 401 | CZ | PHE | 49 | -6.714 | 18.860 | 52.120 | 1.00 14.53 | ACPS |
| MOTA | 402 | C | PHE | 49 | -4.549 | 16.076 | 55.846 | 1.00 11.65 | ACPS |
| MOTA | 403 | 0 | PHE | 49 | -4.059 | 15.616 | 54.809 | 1.00 11.61 | ACPS |
| ATOM | 404 | N | LEU | 50 | -3.852 | 16.805 | 56.71 7 | 1.00 11.42 | ACPS |
| MOTA | 405 | CA | LEU | 50 | -2.454 | 17.140 | 56.489 | 1.00 11.53 | ACPS |
| ATOM | 406 | CB | LEU | 50 | -1.947 | 18.075 | 57.597 | 1.00 12.38 | ACPS |
| ATOM | 407 | CG | LEU | 50 | -0.473 | 18.512 | 57.597 | 1.00 12.32 | ACPS |
| MOTA | 408 | CD1 | LEU | 50 | -0.131 | 19.277 | 56.323 | 1.00 14.40 | ACPS |
| | | | | | | | | | |

| ATOM | 466 | | | | 7.551 | | | 1.00 14.43 | ACPS |
|--------------|------------|-----|--------|----|--------|--------|--------|------------|--------------|
| ATOM | 467 | | E1 GLU | | 7.452 | | | 1.00 12.52 | ACPS |
| ATOM | 468 | | 2 GLU | 58 | 8.343 | 12.641 | 53.905 | 1.00 14.76 | ACPS |
| ATOM | 469 | | GLU | 58 | 5.969 | | 48.903 | 1.00 10.19 | ACPS |
| ATOM | 470 | | GLU | 58 | 6.960 | 9.897 | 48.298 | 1.00 11.04 | ACPS |
| MOTA | 471 | . N | ALA | 59 | 4.773 | 9.742 | 48.765 | | ACPS |
| ATOM | 472 | CA | ALA | 59 | 4.596 | 8.622 | 47.844 | 1.00 10.19 | ACPS |
| MOTA | 473 | CB | ALA | 59 | 3.178 | 8.031 | 47.965 | 1.00 9.73 | ACPS |
| MOTA | 474 | C | ALA | 59 | 4.866 | | 46.415 | 1.00 11.21 | ACPS |
| MOTA | 475 | 0 | ALA | 59 | 5.510 | 8.402 | 45.641 | 1.00 11.07 | ACPS |
| ATOM | 476 | N | PHE | 60 | 4.377 | | 46.071 | 1.00 10.97 | ACPS |
| MOTA | 477 | CA | PHE | 60 | 4.614 | | | 1.00 11.41 | ACPS |
| ATOM | 478 | CB | PHE | 60 | 3.918 | 12.182 | 44.536 | 1.00 11.35 | ACPS |
| ATOM | 479 | CG | PHE | 60 | 4.213 | 12.810 | 43.191 | 1.00 11.93 | ACPS |
| ATOM | 480 | CD | 1 PHE | 60 | 3.492 | 12.439 | 42.057 | 1.00 11.51 | ACPS |
| ATOM | 481 | | 2 PHE | 60 | 5.284 | 13.684 | 43.047 | 1.00 11.60 | ACPS |
| ATOM | 482 | | 1 PHE | 60 | 3.841 | 12.926 | 40.793 | 1.00 12.57 | ACPS |
| ATOM | 483 | | 2 PHE | 60 | 5.641 | 14.174 | 41.794 | 1.00 12.37 | |
| ATOM | 484 | cz | PHE | 60 | 4.921 | 13.794 | 40.671 | 1.00 11.51 | ACPS ACPS |
| ATOM | 485 | C | PHE | 60 | 6.109 | 11.014 | 44.481 | 1.00 10.91 | |
| ATOM | 486 | 0 | PHE | 60 | 6.599 | 10.703 | 43.390 | 1.00 10.31 | ACPS |
| ATOM | 487 | N | SER | 61 | 6.828 | 11.529 | 45.483 | 1.00 11.17 | ACPS |
| ATOM | 488 | CA | SER | 61 | 8.262 | 11.775 | 45.336 | 1.00 11.07 | ACPS |
| ATOM | 489 | СВ | SER | 61 | 8.815 | 12.510 | 46.561 | 1.00 11.40 | ACPS |
| ATOM | 490. | | SER | 61 | 9.026 | 11.642 | 47.660 | 1.00 12.07 | ACPS |
| ATOM | 491 | C | SER | 61 | 9.039 | 10.487 | 45.094 | 1.00 12.07 | ACPS |
| ATOM | 492 | Ō | SER | 61 | 10.102 | 10.508 | 44.476 | 1.00 12.17 | ACPS |
| ATOM | 493 | N | LYS | 62 | 8.513 | 9.365 | 45.583 | 1.00 11.91 | ACPS |
| ATOM | 494 | CA | LYS | 62 | 9.165 | 8.081 | 45.361 | 1.00 11.76 | ACPS |
| ATOM | 495 | CB | LYS | 62 | 8.687 | 7.051 | 46.395 | 1.00 11.72 | ACPS |
| ATOM | 496 | CG | LYS | 62 | 9.172 | 7.377 | 47.836 | 1.00 10.07 | ·~-ACPS. |
| ATOM | 497 | CD | LYS | 62 | 8.584 | 6.402 | 48.888 | 1.00 10.07 | ACPS |
| ATOM | 498 | CE | LYS | 62 | 8.901 | 6.838 | 50.320 | 1.00 10.72 | ACPS |
| ATOM | 499 | NZ | LYS | 62 | 8.292 | 5.910 | 51.344 | 1.00 10.72 | ACPS |
| ATOM | 500 | C | LYS | 62 | 8.875 | | 43.935 | 1.00 11.87 | ACPS ACPS |
| ATOM | 501 | | LYS | 62 | 9.758 | | 43.264 | 1.00 12.36 | ACPS |
| ATOM | 502 | N | ALA | 63 | 7.642 | 7.815 | 43.472 | 1.00 12.30 | |
| ATOM | 503 | CA | ALA | 63 | 7.266 | 7.408 | 42.119 | 1.00 12.11 | ACPS |
| ATOM | 504 | CB | ALA | 63 | 5.751 | 7.567 | 41.914 | 1.00 12.63 | ACPS |
| ATOM | 505 | C | ALA | 63 | 8.033 | 8.259 | 41.105 | 1.00 11.07 | ACPS |
| ATOM | 506 | ō | ALA | 63 | 8.402 | 7.774 | 40.037 | 1.00 13.18 | ACPS |
| ATOM | 507 | N | PHE | 64 | 8.262 | 9.523 | | • | ACPS ACPS |
| ATOM | 508 | CA | PHE | 64 | 8.987 | 10.491 | | 1.00 13.48 | |
| ATOM | 509 | CB | PHE | 64 | 8.856 | 11.878 | 40.628 | 1.00 14.82 | ACPS |
| ATOM | 510 | CG | PHE | 64 | | | 41.290 | 1.00 14.97 | ACPS |
| ATOM | 511 | | PHE | 64 | 9.339 | 13.026 | 40.451 | 1.00 17.08 | ACPS |
| ATOM | 512 | | PHE | | 8.715 | 13.350 | 39.253 | 1.00 17.78 | ACPS |
| ATOM | 513 | | PHE | 64 | 10.402 | 13.809 | 40.885 | 1.00 17.57 | ACPS |
| | | | | 64 | 9.148 | 14.450 | 38.495 | 1.00 18.78 | ACPS |
| ATOM ATOM | 514 515 | | PHE | 64 | 10.838 | 14.904 | 40.137 | 1.00 18.89 | ACPS |
| | 515 | CZ | PHE | 64 | 10.209 | 15.221 | 38.944 | 1.00 18.36 | ACPS |
| MOTA | 516 | C | PHE | 64 | 10.456 | 10.048 | 40.545 | 1.00 14.87 | ACPS |
| MOTA | 517 | 0 | PHE | 64 | 11.136 | 10.290 | 39.547 | 1.00 16.68 | ACPS |
| ATOM | 518 | N | GLY | 65 | 10.941 | 9.423 | 41.615 | 1.00 14.73 | ACPS |
| MOTA | 519 | CA | GLY | 65 | 12.302 | 8.907 | 41.652 | 1.00 14.56 | ACPS |
| MOTA | 520 | С | GLY | 65 | 13.370 | 9.729 | 42.351 | 1.00 14.92 | ACPS |
| MOTA | 521 | 0 | GLY | 65 | 14.542 | 9.351 | 42.348 | 1.00 15.63 | ACPS |
| MOTA | 522 | N | THR | 66 | 12.979 | 10.826 | 42.980 | 1.00 16.03 | ACPS |
| | | | | | | | | | |

| ATON | 1 523 | CA | THR | 66 | 13.945 | 11.700 | 43.643 | 1.00 16.17 | ACPS |
|------|-------|------|-----|----------|--------|--------|--------|------------|------|
| ATO | | | THR | 66 | 13.908 | 13.103 | 43.038 | 1.00 17.57 | ACPS |
| ATON | | | THR | 66 | 12.622 | 13.685 | 43.290 | 1.00 16.98 | ACPS |
| ATON | | | | 66 | 14.150 | 13.056 | 41.531 | 1.00 18.71 | ACPS |
| ATON | | | THR | 66 | 13.770 | 11.912 | 45.140 | 1.00 15.80 | ACPS |
| ATOM | | | THR | 66 | 14.713 | 12.315 | 45.825 | 1.00 15.38 | ACPS |
| ATOM | | | GLY | 67 | 12.572 | 11.652 | 45.649 | 1.00 15.62 | ACPS |
| | | | GLY | 67 | 12.319 | 11.918 | 47.052 | 1.00 15.38 | ACPS |
| MOTA | | | | | | 13.421 | 47.173 | | |
| ATOM | | | GLY | 67 67 | 12.088 | | | 1.00 15.61 | ACPS |
| ATOM | | 0 | GLY | 67 | 12.160 | 14.137 | 46.170 | - | ACPS |
| MOTA | | | ILE | 68 | 11.801 | 13.906 | 48.380 | 1.00 15.09 | ACPS |
| ATOM | | CA | ILE | 68 | 11.580 | 15.332 | 48.598 | 1.00 16.65 | ACPS |
| ATOM | | CB | ILE | 68 | 10.578 | 15.590 | 49.762 | 1.00 15.30 | ACPS |
| ATOM | | | ILE | 68 | 10.508 | 17.089 | 50.063 | 1.00 16.62 | ACPS |
| ATOM | | | ILE | 68 | 9.182 | 15.049 | 49.413 | 1.00 14.84 | ACPS |
| ATOM | | CD1 | | 68 | 8.484 | 15.785 | 48.269 | 1.00 15.16 | ACPS |
| ATOM | 539 | C | ILE | 68 | 12.927 | 15.967 | 48.945 | 1.00 17.33 | ACPS |
| ATOM | 540 | 0 | ILE | 68 | 13.610 | 15.520 | 49.862 | 1.00 18.29 | ACPS |
| ATOM | 541 | N | GLY | 69 | 13.305 | 17.002 | 48.202 | 1.00 18.32 | ACPS |
| ATOM | 542 | CA | GLY | 69 | 14.574 | 17.663 | 48.436 | 1.00 20.27 | ACPS |
| ATOM | 543 | С | GLY | 69 | 14.877 | 18.700 | 47.371 | 1.00 20.85 | ACPS |
| ATOM | 544 | 0 | GLY | 69 | 13.990 | 19.447 | 46.949 | 1.00 20.98 | ACPS |
| ATOM | 545 | N | ALA | 70 | 16.128 | 18.734 | 46.920 | 1.00 22.02 | ACPS |
| ATOM | 546 | CA | ALA | 70 | 16.564 | 19.710 | 45.922 | 1.00 22.94 | ACPS |
| ATOM | 547 | CB | ALA | 70 | 18.064 | 19.575 | 45.690 | 1.00 24.19 | ACPS |
| ATOM | 548 | С | ALA | 70 | 15.834 | 19.655 | 44.582 | 1.00 23.39 | ACPS |
| ATOM | | 0 | ALA | 70 | 15.623 | 20.688 | 43.950 | 1.00 24.35 | ACPS |
| ATOM | | N | GLN | 71 | 15.446 | 18.457 | 44.153 | 1.00 22.46 | ACPS |
| ATOM | | CA | GLN | 71 | 14.765 | 18.289 | 42.871 | 1.00 21.53 | ACPS |
| ATOM | | CB | GLN | 71 | 15.204 | 16.971 | 42.223 | 1.00 23.55 | ACPS |
| ATOM | | CG | GLN | 71 | 16.683 | 16.924 | 41.843 | 1.00 26.32 | ACPS |
| ATOM | | CD | GLN | 71 | 17.185 | 15.512 | 41.591 | 1.00 28.10 | ACPS |
| ATOM | | | GLN | 71 | 17.349 | 14.722 | 42.523 | 1.00 29.41 | ACPS |
| ATOM | | NE2 | | 71 | 17.435 | 15.188 | 40.326 | 1.00 29.15 | ACPS |
| ATOM | | C | GLN | 71 | 13.239 | 18.334 | 42.931 | 1.00 20.50 | ACPS |
| ATOM | | ō | GLN | 71 | 12.580 | 18.424 | 41.891 | 1.00 20.08 | ACPS |
| ATOM | | N | LEU | 72 | 12.668 | 18.287 | 44.132 | 1.00 18.34 | ACPS |
| ATOM | | CA | LEU | 72 | 11.210 | 18.292 | 44.261 | 1.00 16.54 | ACPS |
| ATOM | | CB | LEU | 72 | 10.671 | 16.868 | 44.034 | 1.00 16.42 | ACPS |
| | | CG | LEU | 72 | 9.146 | 16.682 | 44.035 | 1.00 15.69 | ACPS |
| ATOM | • | | LEU | 72 72 | 8.539 | 17.358 | 42.815 | 1.00 16.49 | ACPS |
| ATOM | | | LEU | 72 | 8.811 | 15.186 | 44.032 | 1.00 16.39 | ACPS |
| MOTA | | | | | | | | 1.00 15.95 | ACPS |
| ATOM | | C | LEU | 72 73 | 10.752 | 18.786 | 45.632 | 1.00 15.95 | |
| ATOM | | 0 | LEU | 72 | 11.177 | 18.260 | 46.654 | | ACPS |
| MOTA | | N | SER | 73 | 9.879 | 19.789 | 45.649 | 1.00 15.85 | ACPS |
| ATOM | | CA | SER | 73 | 9.360 | 20.337 | 46.901 | 1.00 15.02 | ACPS |
| MOTA | | CB | SER | 73 | 9.400 | 21.872 | 46.865 | 1.00 16.69 | ACPS |
| MOTA | | OG | SER | 73 | 8.552 | 22.454 | 47.851 | 1.00 18.22 | ACPS |
| ATOM | 571 | С | SER | 73 | 7.920 | 19.896 | 47.122 | 1.00 13.98 | ACPS |
| MOTA | 572 | 0 | SER | 73 | 7.227 | 19.531 | 46.175 | 1.00 14.35 | ACPS |
| ATOM | 573 | N | PHE | 74 | 7.469 | 19.926 | 48.373 | 1.00 13.59 | ACPS |
| ATOM | | CA | PHE | 74 | 6.083 | 19.584 | 48.674 | 1.00 12.78 | ACPS |
| ATOM | | CB | PHE | 74 | 5.802 | 19.731 | 50.177 | 1.00 12.70 | ACPS |
| ATOM | | CG | PHE | 74 | 6.274 | 18.566 | 51.010 | 1.00 13.35 | ACPS |
| ATOM | | CD1 | | 74 | 5.663 | 17.320 | 50.894 | 1.00 14.16 | ACPS |
| ATOM | | CD2 | | 74 | 7.308 | 18.723 | 51.928 | 1.00 15.36 | ACPS |
| ATOM | | CE1 | | 74 | 6.071 | 16.246 | 51.679 | 1.00 13.54 | ACPS |
| AION | 313 | -111 | | , = | 0.071 | 10.240 | J2.07J | | |

| ATOM | 580 | CE2 | PHE | 74 | 7.727 | 17.653 | 52.720 | 1.00 14.73 | ACPS |
|--------------|------------|---------|-----|----------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 581 | CZ | PHE | 74 | 7.104 | 16.412 | 52.592 | 1.00 14.61 | ACPS |
| ATOM | 582 | C | PHE | 74 | 5.172 | 20.539 | 47.894 | 1.00 13.25 | ACPS |
| MOTA | 583 | 0 | PHE | 74 | 4.070 | 20.17 9 | 47.500 | 1.00 13.15 | ACPS |
| MOTA | 584 | N | GLN | 75 | 5.642 | 21.764 | 47.665 | 1.00 13.41 | ACPS |
| MOTA | 585 | CA | GLN | 75 | 4.848 | 22.749 | 46.929 | 1.00 13.12 | ACPS |
| ATOM | 586 | CB | GLN | 75 | 5.437 | 24.152 | 47.124 | 1.00 13.58 | ACPS |
| MOTA | 587 | CG | GLN | 75 | 5.338 | 24.66 7 | 48.545 | 1.00 14.20 | ACPS |
| MOTA | 588 | CD | GLN | 75 | 3.897 | 24.841 | 48.976 | 1.00 15.83 | ACPS |
| MOTA | 589 | 0E1 | GLN | 75 | 3.077 | 25.355 | 48.217 | 1.00 17.10 | ACPS |
| ATOM | 590 | NE2 | GLN | 75 | 3.581 | 24.421 | 50.194 | 1. 0 0 15.26 | ACPS |
| MOTA | 591 | С | GLN | 75 | 4.701 | 22.473 | 45.430 | 1.00 13.39 | ACPS |
| MOTA | 592 | 0 | GLN | 75 | 3.865 | 23.097 | 44.769 | 1.00 14.75 | ACPS |
| ATOM | 593 | N | ASP | 76 | 5.502 | 21.555 | 44.889 | 1.00 13.51 | ACPS |
| ATOM | 594 | CA | ASP | 76 | 5.423 | 21.214 | 43.464 | 1.00 13.36 | ACPS |
| MOTA | 595 | CB | ASP | 76 | 6.760 | 20.670 | 42.950 | 1.00 14.98 | ACPS |
| ATOM | 596 | CG | ASP | 76 | 7.907 | 21.644 | 43.108 | 1.00 15.83 | ACPS |
| MOTA | 597 | | ASP | 76 | 7.682 | 22.872 | 43.049 | 1.00 17.92 | ACPS |
| ATOM | 598 | | ASP | 76 | 9.049 | 21.168 | 43.265 | 1.00 16.55 | ACPS |
| ATOM | 599 | C | ASP | 76 | 4.369 | 20.143 | 43.177 42.016 | 1.00 13.18 | ACPS ACPS |
| MOTA | 600 | 0 | ASP | 76 | 4.138 3.743 | 19.781 19.637 | 44.234 | 1.00 13.17 1.00 12.89 | ACPS |
| ATOM | 601 602 | N CA | ILE | 77 77 | 2.765 | 18.561 | 44.234 | 1.00 12.84 | ACPS |
| ATOM | 603 | CB | ILE | 77 | 3.248 | 17.339 | 44.932 | 1.00 12.04 | ACPS |
| ATOM ATOM | 604 | CG2 | ILE | 77 | 2.405 | 16.122 | 44.608 | 1.00 11.88 | ACPS |
| MOTA | 605 | CG1 | | 77 | 4.722 | 17.053 | 44.638 | 1.00 12.24 | ACPS |
| ATOM | 606 | CD1 | | 77 | 5.413 | 16.211 | 45.724 | 1.00 12.11 | ACPS |
| ATOM | 607 | C | ILE | 77 | 1.414 | 18.999 | 44.664 | 1.00 12.77 | ACPS |
| ATOM | 608 | 0 | ILE | 77 | 1.330 | 19.552 | 45.766 | 1.00 13.68 | ACPS |
| ATOM | 609 | N | GLU | 78 | 0.349 | 18.748 | 43.910 | 1.00 12.53 | ACPS |
| ATOM | 610 | CA | GLU | 78 | -0.975 | 19.130 | 44.373 | 1.00 12.16 | ACPS |
| ATOM | 611 | CB | GLU | 78 | -1.472 | 20.350 | 43.587 | 1.00 12.59 | ACPS |
| ATOM | 612 | CG | GLU | 78 | -2.722 | 20.983 | 44.167 | 1.00 13.40 | ACPS |
| MOTA | 613 | CD | GLU | 78 | -2.987 | 22.339 | 43.559 | 1.00 14.46 | ACPS |
| MOTA | 614 | | GLU | 78 | -3.631 | 22.398 | 42.489 | 1.00 16.38 | ACPS |
| ATOM | 615 | | GLU | 78 | -2.524 | 23.340 | 44.147 | 1.00 15.90 | ACPS |
| ATOM | 616 | C | GLU | 78 | -1.999 | 18.014 | 44.252 | 1.00 11.56 | ACPS |
| ATOM | 617 | 0 | GLU | 78 | -2.145 | 17.402 | 43.198 | 1.00 12.82 | ACPS |
| MOTA | 618 | N | ILE | 79 | -2.704 | 17.748 | 45.344 | 1.00 11.82 | ACPS |
| ATOM | 619 | CA | ILE | 79 | -3.750 | 16.734 | 45.329 | 1.00 12.32 | ACPS |
| ATOM | 620 | CB | ILE | 79 70 | -3.893 | 16.000 | 46.698 46.723 | 1.00 12.41 1.00 12.50 | ACPS ACPS |
| ATOM | 621 | | ILE | 79 70 | -5.201 | 15.191 15.010 | 46.723 | 1.00 12.30 | ACPS |
| ATOM | 622 | | ILE | 79 79 | -2.737 -1.372 | 15.660 | 47.132 | 1.00 12.95 | ACPS |
| MOTA' | 623 624 | CDI | ILE | 79 79 | -5.053 | 17.483 | 45.048 | 1.00 12.33 | ACPS |
| ATOM | 625 | 0 | ILE | 79 | -5.389 | 18.439 | 45.747 | 1.00 13.01 | ACPS |
| ATOM | 626 | N | ARG | 80 | -5.753 | 17.059 | 44.003 | 1.00 12.18 | ACPS |
| MOTA MOTA | 627 | CA | ARG | 80 | -7.037 | 17.649 | 43.633 | 1.00 13.15 | ACPS |
| ATOM | 628 | CB | ARG | 80 | -6.981 | 18.219 | 42.205 | 1.00 13.40 | ACPS |
| ATOM | 629 | CG | ARG | 80 | -5.887 | 19.278 | 41.989 | 1.00 14.66 | ACPS |
| ATOM | 630 | CD | ARG | 80 | -5.931 | 19.884 | 40.592 | 1.00 16.60 | ACPS |
| ATOM | 631 | NE | ARG | 80 | -4.846 | 20.849 | 40.396 | 1.00 16.81 | ACPS |
| ATOM | 632 | CZ | ARG | 80 | -4.588 | 21.471 | 39.248 | 1.00 18.53 | ACPS |
| ATOM | 633 | NH1 | | 80 | -3.581 | 22.331 | 39.175 | 1.00 18.94 | ACPS |
| MOTA | 634 | NH2 | | 80 | -5.331 | 21.240 | 38.173 | 1.00 17.96 | ACPS |
| ATOM | 635 | C | ARG | 80 | -8.061 | 16.516 | 43.701 | 1.00 13.09 | ACPS |
| ATOM | 636 | ō | ARG | 80 | -7.697 | 15.352 | 43.882 | 1.00 13.74 | ACPS |
| | | - | | | | | | | |

| ATOM | 637 | N | LYS | 81 | -9.339 | 16.837 | 43.577 | 1.00 13.78 | ACPS |
|------|-----|-----|-------|----|------------------|--------|---------|------------|------|
| MOTA | 638 | CA | LYS | 81 | -10.349 | 15.789 | 43.610 | 1.00 15.56 | ACPS |
| MOTA | 639 | CB | LYS | 81 | -10.943 | 15.648 | 45.017 | 1.00 17.86 | ACPS |
| MOTA | 640 | CG | LYS | 81 | -11.693 | 16.852 | 45.502 | 1.00 21.01 | ACPS |
| ATOM | 641 | CD | LYS | 81 | -12.183 | 16.669 | 46.939 | 1.00 23.45 | ACPS |
| ATOM | 642 | | LYS | 81 | -12.982 | 17.886 | 47.415 | 1.00 25.03 | ACPS |
| ATOM | 643 | | LYS | 81 | -13.413 | 17.764 | 48.847 | 1.00 28.19 | ACPS |
| ATOM | 644 | | LYS | 81 | -11.446 | 16.080 | 42.612 | | |
| | 645 | | | | | | | 1.00 15.29 | ACPS |
| ATOM | | | LYS | 81 | -11.752 | 17.249 | 42.329 | 1.00 15.96 | ACPS |
| ATOM | 646 | | ASP | 82 | -12.025 | 15.019 | 42.060 | 1.00 14.49 | ACPS |
| ATOM | 647 | | ASP | 82 | -13.102 | 15.191 | 41.102 | 1.00 13.96 | ACPS |
| ATOM | 648 | | ASP | 82 | -13.140 | 14.042 | 40.067 | 1.00 14.55 | ACPS |
| MOTA | 649 | CG | ASP | 82 | -13.516 | 12.682 | 40.660 | 1.00 14.41 | ACPS |
| ATOM | 650 | | . ASP | 82 | -14.130 | 12.609 | 41.738 | 1.00 13.41 | ACPS |
| ATOM | 651 | | ASP | 82 | -13.199 | 11.666 | 40.003 | 1.00 16.39 | ACPS |
| MOTA | 652 | C | ASP | 82 | -14.440 | 15.347 | 41.816 | 1.00 14.59 | ACPS |
| ATOM | 653 | 0 | ASP | 82 | -14.506 | 15.366 | 43.048 | 1.00 13.66 | ACPS |
| MOTA | 654 | N | GLN | 83 | -15.506 | 15.464 | 41.038 | 1.00 16.21 | ACPS |
| ATOM | 655 | CA | GLN | 83 | -16.836 | 15.671 | 41.596 | 1.00 18.34 | ACPS |
| ATOM | 656 | CB | GLN | 83 | -17.809 | 15.984 | 40.454 | 1.00 20.79 | ACPS |
| MOTA | 657 | CG | GLN | 83 | -17.344 | 17.201 | 39.649 | 1.00 25.58 | ACPS |
| ATOM | 658 | CD | GLN | 83 | -18.065 | 17.378 | 38.327 | 1.00 28.04 | ACPS |
| ATOM | 659 | OE1 | GLN | 83 | -17.669 | 18.207 | 37.505 | 1.00 30.79 | ACPS |
| ATOM | 660 | | GLN | 83 | -19.130 | 16.606 | 38.114 | 1.00 29.51 | ACPS |
| ATOM | 661 | C | GLN | 83 | -17.351 | 14.530 | 42.465 | 1.00 18.31 | ACPS |
| ATOM | 662 | 0 | GLN | 83 | -18.304 | 14.707 | 43.225 | 1.00 18.85 | ACPS |
| ATOM | 663 | N | ASN | 84 | -16.722 | 13.366 | 42.363 | 1.00 18.00 | ACPS |
| MOTA | 664 | CA | ASN | 84 | -17.126 | 12.220 | 43.178 | 1.00 18.03 | ACPS |
| ATOM | 665 | CB | ASN | 84 | -16.984 | 10.901 | 42.414 | 1.00 19.80 | ACPS |
| ATOM | 666 | CG | ASN | 84 | -17.959 | 10.776 | 41.269 | 1.00 21.78 | ACPS |
| MOTA | 667 | | ASN | 84 | -19.160 | 10.993 | 41.432 | 1.00 24.79 | ACPS |
| ATOM | 668 | | ASN | 84 | -17.451 | 10.404 | 40.105 | 1.00 23.27 | ACPS |
| ATOM | 669 | C | ASN | 84 | -16.282 | 12.111 | 44.439 | 1.00 16.61 | ACPS |
| ATOM | 670 | ō | ASN | 84 | -16.534 | 11.247 | 45.276 | 1.00 16.49 | ACPS |
| ATOM | 671 | N | GLY | 85 | -15.278 | 12.972 | 44.568 | 1.00 15.58 | ACPS |
| MOTA | 672 | CA | GLY | 85 | -14.424 | 12.920 | | | |
| ATOM | 673 | C | GLY | 85 | -13.153 | | 45.741. | 1.00 14.25 | ACPS |
| | 674 | 0 | GLY | 85 | | 12.107 | 45.539 | 1.00 14.48 | ACPS |
| ATOM | | | | | -12.368 | 11.945 | 46.475 | 1.00 14.65 | ACPS |
| ATOM | 675 | N | LYS | 86 | -12.941 | 11.597 | 44.330 | 1.00 13.84 | ACPS |
| ATOM | 676 | CA | LYS | 86 | -11.741 | 10.810 | 44.042 | 1.00 12.93 | ACPS |
| ATOM | 677 | CB | LYS | 86 | -11.911 | 10.014 | 42.745 | 1.00 13.87 | ACPS |
| MOTA | 678 | CG | LYS | 86 | -10.672 | 9.204 | 42.353 | 1.00 15.94 | ACPS |
| MOTA | 679 | CD | LYS | 86 | -10.789 | 8.679 | 40.926 | 1.00 19.84 | ACPS |
| MOTA | 680 | CE | LYS | 86 | -9.548 | 7.906 | 40.485 | 1.00 20.40 | ACPS |
| MOTA | 681 | NZ | LYS | 86 | -9.484 | 6.545 | 41.078 | 1.00 21.85 | ACPS |
| ATOM | 682 | С | LYS | 86 | -10.534 | 11.730 | 43.883 | 1.00 13.03 | ACPS |
| MOTA | 683 | 0 | LYS | 86 | -10.557 | 12.660 | 43.078 | 1.00 12.98 | ACPS |
| MOTA | 684 | N | PRO | 87 | -9.461 | 11.478 | 44.647 | 1.00 11.91 | ACPS |
| ATOM | 685 | CD | PRO | 87 | -9.315 | 10.444 | 45.694 | 1.00 12.38 | ACPS |
| MOTA | 686 | CA | PRO | 87 | -8.262 | 12.308 | 44.551 | 1.00 11.87 | ACPS |
| ATOM | 687 | CB | PRO | 87 | -7.556 | 12.043 | 45.874 | 1.00 10.81 | ACPS |
| MOTA | 688 | CG | PRO | 87 | -7.838 | 10.568 | 46.090 | 1.00 11.34 | ACPS |
| ATOM | 689 | C | PRO | 87 | -7.3 B 6 | 11.913 | 43.377 | 1.00 11.68 | ACPS |
| ATOM | 690 | ō | PRO | 87 | -7.429 | 10.768 | 42.910 | 1.00 11.62 | ACPS |
| ATOM | 691 | N | TYR | 88 | -6. 61 .5 | 12.882 | 42.895 | 1.00 11.62 | ACPS |
| ATOM | 692 | CA | TYR | 88 | -5.639 | 12.674 | 41.830 | 1.00 11.77 | ACPS |
| ATOM | 693 | CB | TYR | 88 | -6.288 | 12.733 | 40.432 | 1.00 13.03 | ACPS |
| ALON | | | 111 | | · U.200 | 14./33 | 7U,734 | 1.00 13.03 | ACFS |

| ATOM | 69 | 4 C | G TYR | 88 | -6.922 | 14 045 | | | |
|------|-------------|------|--------|----------|----------------|--------|--------|--------------------------|------|
| ATOM | 69! | - | D1 TYR | | -6.188 | | | | ACPS |
| ATOM | 696 | | E1 TYR | | | | | | ACPS |
| ATOM | 69 | | D2 TYR | | -6.787 | | | | ACPS |
| ATOM | 698 | | | | -8.271 | | | | ACPS |
| ATOM | 699 | | | | -8.877 | | | | ACPS |
| ATOM | | | | 88 | -8.131 | | | | ACPS |
| | 700 | | | 88 | -8.728 | | | | ACPS |
| ATOM | 701 | | TYR | 88 | -4.571 | | | | ACPS |
| ATOM | 702 | | TYR | 88 | -4.801 | | | 1.00 11.93 | ACPS |
| ATOM | 703 | | ILE | 89 | -3.385 | | 41.487 | 1.00 11.68 | ACPS |
| ATOM | 704 | | | 89 | -2.302 | | 41.647 | 1.00 12.44 | ACPS |
| ATOM | 705 | | | 89 | -1.037 | 13.765 | 42.199 | 1.00 11.85 | ACPS |
| MOTA | 706 | | | 89 | 0.239 | 14.579 | 41.910 | 1.00 11.95 | ACPS |
| MOTA | 707 | | 1 ILE | 89 | -1.185 | 13.538 | 43.706 | 1.00 11.65 | ACPS |
| ATOM | 708 | | 1 ILE | 89 | -0.021 | 12.751 | 44.320 | 1.00 12.93 | ACPS |
| MOTA | 709 | | ILE | 89 | -1.921 | 15.214 | 40.371 | 1.00 12.52 | ACPS |
| ATOM | 710 | | ILE | 89 | -2.000 | 14.662 | 39.271 | 1.00 13.59 | ACPS |
| ATOM | 711 | | ILE | 90 | -1.527 | 16.470 | 40.539 | 1.00 14.09 | ACPS |
| ATOM | 712 | CA | | 90 | -1.036 | 17.282 | 39.434 | 1.00 14.07 | ACPS |
| MOTA | 713 | CB | | 90 | -1.937 | 18.514 | 39.151 | 1.00 14.62 | ACPS |
| ATOM | 714 | | 2 ILE | 90 | -1.254 | 19.433 | 38.127 | 1.00 15.25 | ACPS |
| MOTA | 715 | CG | | 90 | -3.313 | 18.067 | 38.636 | 1.00 15.67 | ACPS |
| MOTA | 716 | | 1 ILE | 90 | -3.289 | 17.301 | 37.330 | 1.00 16.06 | ACPS |
| ATOM | 717 | C | ILE | 90 | 0.357 | 17.780 | 39.855 | 1.00 14.28 | ACPS |
| ATOM | 718 | 0 | ILE | 90 | 0.514 | 18.342 | 40.940 | 1.00 13.87 | ACPS |
| ATOM | 719 | N | CYS | 91 | 1.362 | 17.520 | 39.016 | 1.00 15.25 | ACPS |
| ATOM | 720 | CA | CYS | 91 | 2.737 | 17.974 | 39.242 | 1.00 15.44 | ACPS |
| ATOM | 721 | CB | CYS | 91 | 3.677 | 16.806 | 39.561 | 1.00 15.30 | ACPS |
| ATOM | 722 | SG | CYS | 91 | 5.404 | 17.317 | 39.841 | 1.00 14.62 | ACPS |
| ATOM | 723 | C | CYS | 91 | 3.139 | 18.606 | 37.916 | 1.00 16.53 | ACPS |
| ATOM | 724 | 0 | CYS | 91 | 3.585 | 17.926 | 36.990 | 1.00 17.19 | ACPS |
| MOTA | 725 | N | THR | 92 | 2.958 | 19.912 | 37.830 | 1.00 17.43 | ACPS |
| ATOM | 726 | CA | THR | 92 | 3.255 | 20.640 | 36.609 | 1.00 19.27 | ACPS |
| ATOM | 727 | CB | THR | 92 | 2.946 | 22.137 | 36.804 | 1.00 20.38 | ACPS |
| ATOM | 728 | OG I | LTHR | 92 | 1.5 5 0 | 22.286 | 37.117 | 1.00 22.97 | ACPS |
| MOTA | 729 | CG2 | THR | 92 | 3.257 | 22.920 | 35.542 | 1.00 21.13 | ACPS |
| ATOM | 730 | C | THR | 92 | 4.685 | 20.436 | 36.102 | 1.00 19.66 | ACPS |
| ATOM | 731 | 0 | THR | 92 | 4.909 | 20.405 | 34.885 | 1.00 19.81 | ACPS |
| MOTA | 732 | N | LYS | 93 | 5.641 | 20.269 | 37.021 | 1.00 19.24 | ACPS |
| MOTA | 733 | CA | LYS | 93 | 7.040 | 20.049 | 36.633 | 1.00 20.40 | ACPS |
| MOTA | 734 | CB | LYS | 93 | 7.950 | 19.936 | 37.869 | 1.00 21.00 | ACPS |
| MOTA | 735 | CG | LYS | 93 | 8.283 | 21.253 | 38.540 | 1.00 23.04 | ACPS |
| ATOM | 736 | CD | LYS | 93 | 9.271 | 21.044 | 39.674 | 1.00 23.13 | ACPS |
| ATOM | 737 | CE | LYS | 93 | 9.5 9 0 | 22.347 | 40.394 | 1.00 25.70 | ACPS |
| MOTA | 738 | NZ | LYS | 93 | 10.683 | 22.160 | 41.393 | 1.00 27.21 | ACPS |
| ATOM | 73 <i>9</i> | С | LYS | 93 | 7.194 | 18.774 | 35.816 | 1.00 19.95 | |
| ATOM | 740 | 0 | LYS | 93 | 8.155 | 18.624 | 35.063 | 1.00 19.63 | ACPS |
| MOTA | 741 | N | LEU | 94 | 6.251 | 17.851 | 35.978 | 1.00 20.99 | ACPS |
| MOTA | 742 | CA | LEU | 94 | 6.279 | 16.575 | 35.264 | | ACPS |
| ATOM | 743 | CB | LEU | 94 | 5.643 | 15.485 | 36.129 | 1.00 22.26 1.00 23.41 | ACPS |
| MOTA | 744 | CG | LEU | 94 | 5.579 | 14.064 | 35.563 | | ACPS |
| ATOM | 745 | | LEU | 94 | 6.980 | | | 1.00 24.26 | ACPS |
| ATOM | 746 | | LEU | 94 | | 13.493 | 35.405 | 1.00 26.39 | ACPS |
| ATOM | 747 | C | LEU | 94 | 4.761 | 13.194 | 36.507 | 1.00 25.01 | ACPS |
| ATOM | 748 | 0 | LEU | | 5.530 | 16.674 | 33.936 | 1.00 23.14 | ACPS |
| ATOM | 749 | N | | 94 05 | 6.110 | 16.499 | 32.862 | 1.00 22.82 | ACPS |
| ATOM | 750 | CA | SER | 95 05 | 4.234 | 16.942 | 34.028 | 1.00 23.89 | ACPS |
| ALON | ,50 | CM | SER | 95 | 3.375 | 17.074 | 32.861 | 1.00 25.33 | ACPS |
| | | | | | | | | | |

| ATOM | 751 | CB | SER | 95 | 3.268 | 15.736 | 32.112 | 1.00 26.52 | ACPS |
|--------------|-----------------|---------|------------|------------|----------------|--------|--------|------------|------|
| ATOM | 752 | OG | SER | 95 | 2.573 | 14.752 | 32.861 | 1.00 27.95 | ACPS |
| MOTA | 753 | C | SER | 95 | 2.002 | 17.531 | 33.354 | 1.00 25.56 | ACPS |
| MOTA | 754 | 0 | SER | 95 | 1.760 | 17.599 | 34.561 | 1.00 24.02 | ACPS |
| ATOM | 755 | N | PRO | 96 | 1.090 | 17.874 | 32.432 | 1.00 26.00 | ACPS |
| MOTA | 756 | CD | PRO | 96 | 1.289 | 18.101 | 30.986 | 1.00 26.52 | ACPS |
| ATOM | 757 | CA | PRO | 96 | -0.240 | 18.324 | 32.853 | 1.00 25.75 | ACPS |
| ATOM | 758 | CB | PRO | 96 | -0.709 | 19.147 | 31.657 | 1.00 26.31 | ACPS |
| ATOM | 759 | CG | PRO | 96 | -0.119 | 18.392 | 30.506 | 1.00 26.75 | ACPS |
| ATOM | 760 | C | PRO | 96 | -1.201 | 17.179 | 33.176 | 1.00 25.06 | ACPS |
| ATOM | 761 | 0 | PRO | 96 | -2.304 | 17.414 | 33.664 | 1.00 25.74 | ACPS |
| ATOM | 762 | N | ALA | 97 | -0.773 | 15.950 | 32.907 | 1.00 24.25 | ACPS |
| MOTA | 763 | CA | ALA | 97 | -1.599 | 14.769 | 33.142 | 1.00 23.20 | ACPS |
| ATOM | 764 | CB | ALA | 97 | -0.967 | 13.555 | 32.479 | 1.00 24.01 | ACPS |
| ATOM | 765 | C | ALA | 97 | -1.872 | 14.463 | 34.611 | 1.00 22.43 | ACPS |
| ATOM | 766 | 0 | ALA | 97 | -1.072 | 14.786 | 35.490 | 1.00 22.83 | ACPS |
| MOTA | 76 7 | N | ALA | 98 | -3.020 | 13.841 | 34.865 | 1.00 21.00 | ACPS |
| ATOM | 768 | CA | ALA | 98 | -3.411 | 13.462 | 36.215 | 1.00 19.60 | ACPS |
| MOTA | 769 | CB | ALA | 98 | -4.914 | 13.140 | 36.259 | 1.00 19.71 | ACPS |
| MOTA | 770 | С | ALA | 98 | -2.597 | 12.232 | 36.601 | 1.00 18.50 | ACPS |
| ATOM | 771 | 0 | ALA | 98 | -2.426 | 11.313 | 35.796 | 1.00 19.87 | ACPS |
| ATOM | 772 | N | VAL | 99 | -2.084 | 12.231 | 37.826 | 1.00 15.98 | ACPS |
| MOTA | 773 | CA | VAL | 99 | -1.299 | 11.120 | 38.346 | 1.00 14.14 | ACPS |
| ATOM | 774 | CB | VAL | 99 | -0.042 | 11.661 | 39.041 | 1.00 15.01 | ACPS |
| MOTA | 775 | CG1 | VAL | 99 | 0.630 | 10.575 | 39.854 | 1.00 15.26 | ACPS |
| MOTA | 776 | CG2 | VAL | 99 | 0.909 | 12.221 | 37.990 | 1.00 14.69 | ACPS |
| ATOM | 777 | C | VAL | 99 | -2.192 | 10.357 | 39.336 | 1.00 13.62 | ACPS |
| MOTA | 778 | 0 | VAL | 99 | -2.935 | 10.971 | 40.098 | 1.00 14.19 | ACPS |
| ATOM | 77 9 | N | HIS | 100 | -2.132 | 9.029 | 39.306 | 1.00 12.36 | ACPS |
| MOTA | 780 | CA | HIS | 100 | -2.949 | 8.192 | 40.178 | 1.00 12.74 | ACPS |
| MOTA | 781 | CB | HIS | 100 | -2.894 | 6.741 | 39.708 | 1.00 13.48 | ACPS |
| MOTA | 782 | CG | HIS | 100 | -3.505 | 6.514 | 38.362 | 1.00 14.92 | ACPS |
| MOTA | 783 | | HIS | 100 | -2.938 | 6.353 | 37.143 | 1.00 15.96 | ACPS |
| ATOM | 784 | | HIS | 100 | -4.868 | 6.432 | 38.165 | 1.00 15.90 | ACPS |
| ATOM | 785 | | HIS | 100 | -5.113 | 6.232 | 36.883 | 1.00 17.29 | ACPS |
| ATOM | 786 | | HIS | 100 | -3.960 | 6.181 | 36.241 | 1.00 15.85 | ACPS |
| MOTA | 787 | C | HIS | 100 | -2.513 | 8.233 | 41.630 | 1.00 12.24 | ACPS |
| ATOM | 788 | 0 | HIS | 100 | -1.328 | 8.140 | 41.927 | 1.00 12.33 | ACPS |
| ATOM | 789 | N | VAL | 101 | -3.487 | 8.363 | 42.525 | 1.00 11.72 | ACPS |
| ATOM | 790 | CA | VAL | 101 | -3.217 | 8.365 | 43.958 | 1.00 11.15 | ACPS |
| ATOM | 791 | CB | VAL | 101 | -2.899 | 9.811 | 44.477 | 1.00 11.69 | ACPS |
| MOTA | 792 | | VAL | 101 | -4.142 | 10.694 | 44.373 | 1.00 12.75 | ACPS |
| ATOM | 793 | | VAL | 101 | -2.391 | | | 1.00 12.34 | ACPS |
| ATOM | 794 | C | VAL | 101 | -4.430 | 7.815 | 44.725 | 1.00 10.53 | ACPS |
| ATOM | 795 | 0 | VAL | 101 | -5.565 | 7.914 | 44.253 | 1.00 10.71 | ACPS |
| ATOM | 796 | N | SER | 102 | -4.174 | 7.176 | 45.871 | 1.00 9.38 | ACPS |
| ATOM | 797 798 | CA | SER SER | 102 | -5.243 | 6.698 | 46.748 | 1.00 9.83 | ACPS |
| ATOM ATOM | 799 | CB | SER | 102 102 | -5.574 | 5.218 | 46.517 | 1.00 10.13 | ACPS |
| | | og C | | | -6.713 | 4.863 | 47.295 | 1.00 9.75 | ACPS |
| MOTA | 800 | 0 | SER | 102 | -4.782 | 6.906 | 48.192 | 1.00 9.45 | ACPS |
| ATOM | 801 | | SER | 102 | -3.608 | 6.730 | 48.493 | 1.00 10.30 | ACPS |
| ATOM | 802 | N | ILE | 103 | -5. 712 | 7.277 | 49.071 | 1.00 9.23 | ACPS |
| ATOM | 803 | CA | ILE | 103 | -5.417 | 7.563 | 50.474 | 1.00 9.67 | ACPS |
| ATOM | 804 | CB | ILE | 103 | -5.683 | 9.063 | 50.774 | 1.00 9.72 | ACPS |
| ATOM | 805 | CG2 | | 103 | -5.495 | 9.382 | 52.283 | 1.00 8.94 | ACPS |
| ATOM | 806 | CG1 | | 103 | -4.778 | 9.912 | 49.885 | 1.00 10.44 | ACPS |
| MOTA | 807 | CD1 | 1LE | 103 | -5.088 | 11.421 | 49.938 | 1.00 11.38 | ACPS |
| | | | | | | | | | |

| ATOM | 808 | | ILE | 103 | -6.2 9 9 | 6.728 | 51.388 | 1.00 9.74 | ACPS |
|------|-----|-----|-------|-----|--------------------|--------|--------|------------|------|
| ATOM | 809 | 0 | ILE | 103 | -7.447 | 6.432 | 51.041 | 1.00 9.47 | ACPS |
| ATOM | 810 | N | THR | 104 | -5.751 | 6.334 | 52.541 | 1.00 9.43 | ACPS |
| ATOM | 811 | CA | THR | 104 | -6.5 07 | 5.567 | 53.537 | 1.00 9.07 | ACPS |
| MOTA | 812 | CB | THR | 104 | -6.323 | 4.034 | 53.329 | 1.00 9.49 | ACPS |
| ATOM | 813 | OG: | 1 THR | 104 | -7.164 | 3.312 | 54.246 | 1.00 10.14 | ACPS |
| ATOM | 814 | CG: | 2 THR | 104 | -4.878 | 3.617 | 53.528 | 1.00 8.69 | ACPS |
| ATOM | 815 | C | THR | 104 | -6.067 | 5.976 | 54.949 | 1.00 9.89 | ACPS |
| ATOM | 816 | | THR | 104 | -4.89 6 | 6.283 | 55.174 | 1.00 9.73 | ACPS |
| ATOM | 817 | | HIS | 105 | -7.006 | 5.978 | 55.891 | 1.00 10.13 | ACPS |
| ATOM | 818 | | HIS | 105 | -6.734 | 6.384 | 57.266 | 1.00 10.93 | ACPS |
| ATOM | 819 | CB | HIS | 105 | -7.632 | 7.572 | 57.622 | 1.00 11.25 | ACPS |
| MOTA | 820 | CG | HIS | 105 | -7.371 | 8.805 | 56.817 | 1.00 11.60 | ACPS |
| ATOM | 821 | | HIS | 105 | -7.921 | 9.254 | 55.663 | 1.00 13.08 | ACPS |
| ATOM | 822 | | HIS | 105 | -6.442 | 9.749 | 57.192 | 1.00 11.93 | ACPS |
| ATOM | 823 | | HIS | 105 | -6.427 | 10.729 | 56.305 | 1.00 11.86 | ACPS |
| ATOM | 824 | | HIS | 105 | -7.315 | 10.451 | 55.366 | 1.00 12.18 | ACPS |
| ATOM | 825 | C | HIS | 105 | -6.98 6 | 5.299 | 58.314 | 1.00 11.03 | ACPS |
| ATOM | 826 | ō | HIS | 105 | -7.88 8 | 4.471 | 58.165 | 1.00 12.54 | ACPS |
| ATOM | 827 | N | THR | 106 | -6.165 | 5.309 | 59.367 | 1.00 11.51 | ACPS |
| ATOM | 828 | CA | THR | 106 | -6.349 | 4.411 | 60.509 | 1.00 11.59 | ACPS |
| ATOM | 829 | СВ | THR | 106 | -5.289 | 3.270 | 60.620 | 1.00 11.24 | ACPS |
| ATOM | 830 | | THR | 106 | -4.065 | 3.780 | 61.169 | 1.00 11.20 | ACPS |
| ATOM | 831 | CG2 | | 106 | -5.017 | 2.634 | 59.261 | 1.00 12.65 | ACPS |
| ATOM | 832 | C | THR | 106 | -6.225 | 5.273 | 61.771 | 1.00 12.23 | ACPS |
| MOTA | 833 | ō | THR | 106 | -6.002 | 6.482 | 61.692 | 1.00 12.54 | ACPS |
| ATOM | 834 | N | LYS | 107 | -6.364 | 4.634 | 62.929 | 1.00 12.39 | ACPS |
| ATOM | 835 | CA | LYS | 107 | -6.2 69 | 5.295 | 64.229 | 1.00 12.12 | ACPS |
| ATOM | 836 | CB | LYS | 107 | -6.473 | 4.242 | 65.326 | 1.00 12.29 | ACPS |
| ATOM | 837 | CG | LYS | 107 | -5.3 79 | 3.146 | 65.280 | 1.00 13.31 | ACPS |
| ATOM | 838 | CD | LYS | 107 | -5.653 | 1.939 | 66.203 | 1.00 14.42 | ACPS |
| ATOM | 839 | CE | LYS | 107 | -4.660 | 0.799 | 65.876 | 1.00 15.82 | ACPS |
| ATOM | 840 | NZ | LYS | 107 | -4.895 | -0.473 | 66.648 | 1.00 18.55 | ACPS |
| ATOM | 841 | С | LYS | 107 | -4.93 6 | 5.998 | 64.490 | 1.00 12.43 | ACPS |
| ATOM | 842 | 0 | LYS | 107 | -4.87 4 | 6.970 | 65.263 | 1.00 14.30 | ACPS |
| MOTA | 843 | N | GLU | 108 | -3.8 71 | 5.516 | 63.857 | 1.00 11.38 | ACPS |
| ATOM | 844 | CA | GLU | 108 | -2.540 | 6.061 | 64.099 | 1.00 11.08 | ACPS |
| ATOM | 845 | CB | GLU | 108 | -1.692 | 4.997 | 64.823 | 1.00 10.76 | ACPS |
| MOTA | 846 | CG | GLU | 108 | -1.32 0 | 3.790 | 63.936 | 1.00 11.72 | ACPS |
| ATOM | 847 | CD | GLU | 108 | -0.835 | 2.550 | 64.706 | 1.00 11.82 | ACPS |
| ATOM | 848 | OE1 | GLU | 108 | -0.047 | 2.673 | 65.664 | 1.00 12.16 | ACPS |
| ATOM | 849 | OE2 | GLU | 108 | -1.224 | 1.420 | 64.329 | 1.00 11.39 | ACPS |
| ATOM | 850 | С | GLU | 108 | -1.788 | 6.517 | 62.858 | 1.00 10.37 | ACPS |
| ATOM | 851 | 0 | GLU | 108 | -0.76 9 | 7.193 | 62.977 | 1.00 10.85 | ACPS |
| ATOM | 852 | N | TYR | 109 | -2.292 | 6.164 | 61.676 | 1.00 10.03 | ACPS |
| ATOM | 853 | CA | TYR | 109 | -1.608 | 6.482 | 60.421 | 1.00 9.03 | ACPS |
| MOTA | 854 | CB | TYR | 109 | -1.061 | 5.195 | 59.757 | 1.00 10.14 | ACPS |
| ATOM | 855 | CG | TYR | 109 | -0.074 | 4.364 | 60.537 | 1.00 9.25 | ACPS |
| ATOM | 856 | CD1 | | 109 | 1.091 | 4.927 | 61.043 | 1.00 9.05 | ACPS |
| ATOM | 857 | | TYR | 109 | 2.032 | 4.157 | 61.725 | 1.00 10.07 | ACPS |
| ATOM | 858 | | TYR | 109 | -0.28 3 | 2.996 | 60.730 | 1.00 10.49 | ACPS |
| ATOM | 859 | CE2 | | 109 | 0.649 | 2.217 | 61.410 | 1.00 10.45 | ACPS |
| ATOM | 860 | CZ | TYR | 109 | 1.807 | 2.809 | 61.902 | 1.00 10.01 | ACPS |
| ATOM | 861 | OH | TYR | 109 | 2.753 | 2.042 | 62.546 | 1.00 11.02 | ACPS |
| ATOM | 862 | C | TYR | 109 | -2.48 7 | 7.101 | 59.343 | 1.00 11.45 | ACPS |
| ATOM | 863 | 0 | TYR | 109 | -3.70 8 | 6.991 | 59.343 | 1.00 9.01 | |
| | 864 | N | ALA | | | | | | ACPS |
| ATOM | 004 | 7.4 | TUM | 110 | -1.825 | 7.735 | 58.381 | 1.00 9.15 | ACPS |
| | | | | | | | | | |

| ATOM | 865 | | | | -2.475 | | 57.162 | 1.00 10.18 | ACPS |
|--------------|--------------|---------|------------|------------|------------------|--------|--------|------------|-------------|
| ATOM | 866 | | | | -2.489 | | | | ACPS |
| ATOM | 867 | | ALA | 110 | -1.529 | | 56.110 | 1.00 8.99 | ACPS |
| MOTA | 868 | | ALA | 110 | -0.322 | 7.843 | | 1.00 10.23 | ACPS |
| ATOM | 869 | | ALA | 111 | -2.06 7 | 6.776 | 55.209 | 1.00 9.06 | ACPS |
| ATOM | 870 | | | 111 | -1.255 | 6.109 | 54.181 | 1.00 9.24 | ACPS |
| ATOM | 871 | | ALA | 111 | -1.319 | 4.577 | 54.371 | 1.00 9.27 | ACPS |
| ATOM | 872 | C | ALA | 111 | -1.710 | 6.462 | 52.773 | 1.00 9.10 | ACPS |
| ATOM | 873 | 0 | ALA | 111 | -2.877 | 6.780 | 52.551 | 1.00 9.14 | ACPS |
| MOTA | 874 | N | ALA | 112 | -0.782 | 6.399 | 51.822 | 1.00 9.52 | ACPS |
| ATOM | 875 | CA | ALA | 112 | -1.107 | 6.713 | 50.434 | 1.00 9.40 | ACPS |
| MOTA | 876 | CB | ALA | 112 | -0.973 | 8.219 | 50.190 | 1.00 10.40 | ACPS |
| MOTA | 877 | | ALA | 112 | -0.202 | 5.984 | 49.462 | 1.00 9.11 | ACPS |
| ATOM | 878 | | ALA | 112 | 0.890 | 5.548 | 49.814 | 1.00 9.27 | ACPS |
| MOTA | 879 | N | GLN | 113 | -0.680 | 5.843 | 48.233 | 1.00 10.03 | ACPS |
| MOTA | 880 | CA | GLN | 113 | 0.124 | 5.246 | 47.171 | 1.00 10.71 | ACPS |
| MOTA | 881 | CB | GLN | 113 | -0.221 | 3.768 | 46.949 | 1.00 12.50 | ACPS |
| ATOM | 882 | | GLN | 113 | -1.607 | 3.525 | 46.382 | 1.00 14.15 | ACPS |
| ATOM | 883 | | GLN | 113 | -1.910 | 2.053 | 46.181 | 1.00 16.57 | ACPS |
| MOTA | 884 | | l GLN | 113 | -2.978 | 1.699 | 45.686 | 1.00 17.95 | ACPS |
| ATOM | 885 | | 2 GLN | 113 | -0.978 | 1.187 | 46.581 | 1.00 19.32 | ACPS |
| ATOM | 886 | С | GLN | 113 | -0.088 | 6.047 | 45.884 | 1.00 10.42 | ACPS |
| MOTA | 887 | 0 | GLN | 113 | -1.121 | 6.698 | 45.701 | 1.00 11.38 | ACPS |
| ATOM | 888 | N | VAL | 114 | 0.905 | 5.998 | 45.002 | 1.00 10.88 | ACPS |
| MOTA | 889 | CA | VAL | 114 | 0.872 | 6.727 | 43.742 | 1.00 11.50 | ACPS |
| ATOM | 890 | CB | VAL | 114 | 1.770 | 8.002 | 43.834 | 1.00 12.48 | ACPS |
| ATOM | 891 | | l VAL | 114 | 1.994 | 8.613 | 42.444 | 1.00 12.51 | ACPS |
| ATOM | 892 | | VAL | 114 | 1.144 | 9.013 | 44.779 | 1.00 11.66 | ACPS |
| ATOM | 893 | C | VAL | 114 | 1.409 | 5.888 | 42.589 | 1.00 11.78 | ACPS |
| ATOM | 894 | 0 | VAL | 114 | 2.295 | 5.055 | 42.772 | 1.00 11.30 | ACPS |
| ATOM | 895 | N | VAL | 115 | 0.839 | 6.099 | 41.405 | 1.00 12.16 | ACPS |
| ATOM | 896 | CA | VAL | 115 | 1.322 | 5.454 | 40.195 | 1.00 12.60 | ACPS |
| ATOM | 897 | CB | VAL | 115 | 0.426 | 4.301 | 39.706 | 1.00 12.42 | ACPS |
| ATOM | 898 | | VAL | 115 | 0.957 | 3.778 | 38.377 | 1.00 14.70 | ACPS |
| ATOM | 899 | | VAL | 115 | 0.388 | 3.172 | 40.736 | 1.00 12.57 | ACPS |
| ATOM | 900 | C | VAL | 115 | 1.364 | 6.525 | 39.109 | 1.00 12.96 | A:CPS |
| ATOM ATOM | 901 902 | 0 | VAL | 115 | 0.351 | 7.167 | 38.821 | 1.00 13.15 | ACPS |
| ATOM | 903 | N CA | ILE | 116 116 | 2.547 | 6.732 | 38.534 | 1.00 13.59 | A.CPS |
| ATOM | 904 | CB | ILE | 116 | 2.736 | 7.708 | 37.454 | 1.00 15.01 | ACPS |
| ATOM | 905 | | ILE | 116 | 4.044 | 8.514 | 37.619 | 1.00 15.13 | ACPS |
| ATOM | 906 | | ILE | 116 | 4.252 | 9.422 | 36.391 | 1.00 15.76 | ACPS |
| ATOM | 907 | | ILE | 116 | 4.011 5.326 | | 38.901 | 1.00 14.74 | ACPS |
| ATOM | 908 | C | ILE | 116 | 2.881 | 10.082 | 39.168 | 1.00 15.57 | ACPS |
| ATOM | 909 | 0 | ILE | 116 | | 6.907 | 36.164 | 1.00 16.45 | ACPS |
| ATOM | 910 | N | GLU | 117 | 3.750 | 6.032 | 36.076 | 1.00 16.35 | ACPS |
| ATOM | 911 | CA | GLU | 117 | 2.054 | 7.205 | 35.165 | 1.00 18.81 | ACPS |
| ATOM | 912 | СВ | GLU | 117 | 2.142 | 6.481 | 33.894 | 1.00 21.39 | ACPS |
| ATOM | 913 | CG | GLU | 117 | 0.760 | 6.363 | 33.245 | 1.00 22.18 | ACPS |
| ATOM | 914 | CD | GLU | 117 | -0.272 -1.560 | 5.679 | 34.124 | 1.00 23.46 | ACPS |
| ATOM | 915 | | GLU | 117 | -1.580 | 5.358 | 33.391 | 1.00 24.48 | ACPS |
| ATOM | 916 | | GLU | 117 | -1.582 -2.550 | 4.373 | 32.622 | 1.00 25.10 | ACPS |
| MOTA | 917 | C | GLU | 117 | | 6.092 | 33.580 | 1.00 25.49 | ACPS |
| ATOM | 918 | 0 | GLU | | 3.097 | 7.186 | 32.938 | 1.00 23.33 | ACPS |
| MOTA | 919 | N | ALA | 117 | 3.386 | 8.367 | 33.101 | 1.00 23.55 | ACPS |
| ATOM | 920 | CA | | 118 | 3.596 | 6.460 | 31.943 | 1.00 25.38 | ACPS |
| ATOM | 920 921 | CB | ALA ALA | 118 | 4.516 | 7.055 | 30.979 | 1.00 27.43 | ACPS |
| ATON | 9 2 1 | CD | THE | 118 | 4.977 | 6.002 | 29.985 | 1.00 27.34 | ACPS |
| | | | | | | | | | |

| ATOM | 922 | | | 118 | 3.841 | 8.208 | 30.244 | 1.00 28.57 | ACPS |
|------|-----|-----|--------|-----|---------|--------|--------|------------|------|
| ATOM | 923 | | rı ala | 118 | 2.598 | 8.169 | 30.110 | 1.00 29.57 | ACPS |
| ATOM | 924 | | rz ala | 118 | 4.563 | 9.133 | 29.800 | 1.00 30.29 | ACPS |
| ATOM | 925 | | нон | 1 | 8.184 | | 66.146 | 1.00 24.49 | WAT |
| MOTA | 926 | | HOH | 2 | 8.785 | 8.855 | 56.929 | 1.00 23.58 | WAT |
| MOTA | 927 | | HOH | 3 | -6.634 | 6.371 | 40.520 | 1.00 13.40 | WAT |
| ATOM | 928 | 3 0 | HOH | 4 | 6.850 | 6.588 | 56.334 | 1.00 12.56 | WAT |
| MOTA | 929 | 0 | HOH | 5 | -8.045 | 6.689 | 43.987 | 1.00 13.42 | WAT |
| MOTA | 930 | 0 | HOH | 6 | -5.322 | 9.243 | 59.567 | 1.00 14.25 | WAT |
| MOTA | 931 | . 0 | HOH | 7 | -8.408 | 6.897 | 46.767 | 1.00 10.54 | WAT |
| ATOM | 932 | 0 | HOH | 8 | 0.163 | 8.272 | 65.337 | 1.00 14.13 | WAT |
| ATOM | 933 | 0 | HOH | 9 | -14.561 | 9.350 | 40.005 | 1.00 16.00 | WAT |
| MOTA | 934 | | HOH | 10 | 5.984 | 9.787 | 56.562 | 1.00 12.10 | WAT |
| ATOM | 935 | 0 | HOH | 11 | 9.603 | 20.654 | 50.362 | 1.00 18.90 | WAT |
| ATOM | 936 | 0 | HOH | 12 | 9.199 | 12.001 | 56.416 | 1.00 20.43 | WAT |
| ATOM | 937 | 0 | HOH | 13 | -5.501 | 13.397 | | 1.00 13.06 | WAT |
| MOTA | 938 | 0 | HOH | 14 | -2.767 | 25.961 | 44.622 | 1.00 17.37 | WAT |
| ATOM | 939 | 0 | HOH | 15 | 1.460 | 20.979 | 40.473 | 1.00 16.78 | WAT |
| ATOM | 940 | 0 | HOH | 16 | -6.412 | 20.992 | 45.756 | 1.00 19.74 | WAT |
| ATOM | 941 | 0 | HOH | 17 | -6.145 | 9.042 | 41.305 | 1.00 12.90 | TAW |
| ATOM | 942 | 0 | HOH | 18 | -0.223 | 24.078 | 42.670 | 1.00 18.93 | TAW |
| ATOM | 943 | 0 | HOH | 19 | -7.596 | 19.455 | 37.156 | 1.00 19.34 | WAT |
| ATOM | 944 | 0 | HOH | 20 | -5.063 | 33.496 | 51.266 | 1.00 22.07 | WAT |
| MOTA | 945 | 0 | HOH | 21 | -1.492 | 0.933 | 67.571 | 1.00 14.90 | TAW |
| ATOM | 946 | 0 | HOH | 22 | 10.843 | 7.091 | 38.836 | 1.00 23.19 | TAW |
| ATOM | 947 | 0 | HOH | 23 | 1.577 | 14.422 | 68.706 | 1.00 24.82 | TAW |
| ATOM | 948 | 0 | HOH | 24 | -7.606 | 8.898 | 61.270 | 1.00 18.79 | TAW |
| ATOM | 949 | 0 | HOH | 25 | 0.081 | 9.327 | 35.513 | 1.00 22.45 | WAT |
| MOTA | 950 | 0 | HOH | 26 | -6.295 | 18.339 | 48.365 | 1.00 15.49 | WAT |
| ATOM | 951 | 0 | HOH | 27 | -0.673 | 19.887 | 66.759 | 1.00 21.01 | WAT |
| MOTA | 952 | 0 | HOH | 28 | 2.234 | 22.708 | 42.588 | 1.00 18.21 | WAT |
| ATOM | 953 | 0 | HOH | 29 | 5.866 | 5.790 | 62.516 | 1.00 18.49 | WAT |
| ATOM | 954 | 0 | HOH | 30 | 0.991 | 15.961 | 36.660 | 1.00 18.35 | WAT |
| ATOM | 955 | 0 | HOH | 31 | -6.406 | 9.357 | 38.563 | 1.00 20.48 | WAT |
| ATOM | 956 | | HOH | 32 | -11.957 | 11.623 | 37.352 | 1.00 24.33 | WAT |
| ATOM | 957 | 0 | HOH | 33 | -10.389 | 14.434 | 49.725 | 1.00 27.42 | WAT. |
| ATOM | 958 | 0 | нон | 34 | -4.448 | 20.165 | 63.854 | 1.00 24.32 | WAT |
| ATOM | 959 | 0 | HOH | 35 | 1.450 | 2.725 | 43.903 | 1.00 20.38 | WAT |
| ATOM | 960 | 0 | нон | 36 | -9.847 | 19.977 | 43.739 | 1.00 23.75 | WAT |
| ATOM | 961 | 0 | нон | 37 | -4.274 | 35.006 | 45.404 | 1.00 20.66 | WAT |
| MOTA | 962 | 0 | нон | 38 | -0.833 | 22.659 | 40.326 | 1.00 19.80 | WAT |
| MOTA | 963 | 0 | НОН | 39 | -10.345 | 18.568 | 67.239 | 1.00 20.80 | WAT |
| MOTA | 964 | 0 | HOH | 40 | -8.477 | 13.551 | 55.975 | 1.00 26.24 | WAT |
| ATOM | 965 | 0 | нон | 41 | -5.655 | 29.371 | 49.873 | 1.00 28.51 | WAT |
| MOTA | 966 | 0 | НОН | 42 | -10.675 | 16.934 | 50.659 | 1.00 24.92 | WAT |
| MOTA | 967 | 0 | HOH | 43 | -12.936 | 12.520 | 51.596 | 1.00 27.30 | WAT |
| ATOM | 968 | 0 | нон | 44 | 5.317 | 21.159 | 39.730 | 1.00 21.12 | WAT |
| ATOM | 969 | 0 | нон | 45 | -16.788 | 9.865 | 48.461 | 1.00 26.54 | WAT |
| ATOM | 970 | 0 | НОН | 46 | -11.077 | 6.886 | 57.927 | 1.00 23.02 | WAT |
| ATOM | 971 | 0 | HOH | 47 | 8.239 | 21.236 | 62.377 | 1.00 34.53 | WAT |
| ATOM | 972 | 0 | нон | 48 | -12.230 | 29.900 | 51.577 | 1.00 21.86 | WAT |
| ATOM | 973 | 0 | HOH | 49 | 14.440 | 16.080 | 45.556 | 1.00 23.96 | WAT |
| ATOM | 974 | 0 | НОН | 50 | 12.861 | 21.772 | 39.431 | 1.00 30.68 | WAT |
| ATOM | 975 | 0 | HOH | 51 | -14.091 | 19.163 | 60.526 | 1.00 27.55 | WAT |
| ATOM | 976 | 0 | HOH | 52 | 6.663 | 27.800 | 61.179 | 1.00 32.84 | TAW |
| ATOM | 977 | 0 | HOH | 53 | -11.635 | 27.871 | 53.345 | 1.00 31.03 | TAW |
| ATOM | 978 | 0 | нон | 54 | -6.997 | 7.591 | 67.044 | 1.00 25.57 | WAT |
| | | | | | | | | | |

| ATOM | 979 | | HOH | 55 | 5.799 | 6.629 | 59.843 | 1.00 16.31 | WAT |
|------|------|-----|-----|------------|------------------|--------|--------|------------|-------|
| MOTA | 980 | | HOH | 56 | 2.012 | 25.703 | 66.142 | 1.00 35.32 | TAW |
| MOTA | 981 | L O | HOH | 57 | 0.121 | 2.727 | 31.610 | 1.00 42.03 | WAT |
| MOTA | 982 | 2 0 | HOH | 58 | 1.534 | 10.328 | 32.415 | 1.00 41.42 | WAT |
| ATOM | 983 | 0 | HOH | 59 | -16.524 | 4.165 | 56.298 | | WAT |
| MOTA | 984 | 0 | HOH | 60 | -13.305 | 16.632 | 64.615 | | WAT |
| MOTA | 985 | 0 | HOH | 61 | -12.177 | 16.550 | 67.442 | 1.00 20.64 | WAT |
| ATOM | 986 | 0 | HOH | 62 | -14.009 | 9.985 | | 1.00 25.38 | WAT |
| ATOM | 987 | 0 | HOH | 63 | -9.900 | 9.225 | | 1.00 23.49 | WAT |
| ATOM | 988 | 0 | HOH | 64 | -6.771 | | | 1.00 21.83 | WAT |
| ATOM | 989 | 0 | HOH | 65 | -2.713 | | | 1.00 24.39 | WAT |
| MOTA | 990 | 0 | нон | 66 | -7.980 | 17.897 | | 1.00 22.87 | WAT |
| ATOM | 991 | 0 | нон | 67 | -13.405 | 7.809 | 38.191 | 1.00 26.90 | WAT |
| ATOM | 992 | | HOH | 68 | -4.952 | 28.402 | 44.638 | 1.00 33.63 | TAW |
| ATOM | 993 | 0 | нон | 69 | -2.685 | 3.686 | 68.288 | 1.00 35.03 | WAT |
| ATOM | 994 | | нон | 70 | 8.512 | 9.048 | 60.830 | 1.00 28.65 | |
| ATOM | 995 | o | нон | 71 | -1.486 | 18.163 | 62.740 | 1.00 28.65 | WAT |
| ATOM | 996 | 0 | нон | 72 | 5.603 | 18.678 | 70.084 | 1.00 32.43 | TAW |
| MOTA | 997 | ō | нон | 73 | -7.54 7 | 29.689 | 51.621 | 1.00 28.38 | WAT |
| ATOM | 998 | ō | НОН | 74 | 10.855 | 19.331 | 52.981 | 1.00 25.41 | WAT |
| ATOM | 999 | ŏ | НОН | 75 | -11.689 | 10.901 | 61.337 | 1.00 28.05 | WAT |
| ATOM | 1000 | ō | нон | 76 | -0.166 | 23.981 | 38.303 | 1.00 28.27 | TAW |
| ATOM | 1001 | ō | нон | 77 | -11.224 | 22.643 | 66.111 | 1.00 33.92 | TAW |
| ATOM | 1002 | ō | нон | 78 | 15.942 | 18.609 | 39.466 | | TAW |
| ATOM | 1003 | ō | нон | 79 | -9.721 | 15.254 | 57.360 | 1.00 35.09 | WAT |
| ATOM | 1004 | ō | нон | 80 | -9.623 | 11.467 | 57.685 | 1.00 23.81 | WAT |
| ATOM | 1005 | ō | нон | 81 | -10.600 | 4.395 | 59.079 | 1.00 26.57 | WAT |
| ATOM | 1006 | ŏ | нон | 82 | -8.498 | 10.896 | | 1.00 26.62 | WAT |
| ATOM | 1007 | o | нон | 83 | -2.753 | 18.652 | 38.078 | 1.00 35.64 | TAW |
| ATOM | 1008 | o | нон | 84 | 9.568 | 24.455 | 65.536 | 1.00 26.51 | WAT |
| ATOM | 1009 | o | нон | 85 | 19.835 | 12.684 | 43.921 | 1.00 31.56 | WAT |
| ATOM | 1010 | õ | нон | 86 | 13.338 | 21.812 | 45.040 | 1.00 35.96 | WAT |
| ATOM | 1011 | Ö | нон | 87 | 11.096 | 20.032 | 46.003 | 1.00 39.76 | WAT |
| ATOM | 1012 | ō | нон | 88 | 3.720 | 23.855 | 59.974 | 1.00 34.99 | WAT |
| ATOM | 1013 | ŏ | нон | 89 | -1.224 | 22.461 | 40.646 | 1.00 31.59 | WAT |
| ATOM | 1014 | Ö | HOH | 90 | -7.691 | 9.770 | 66.261 | 1.00 34.76 | TAW |
| ATOM | 1015 | o | нон | 91 | 17.406 | | 63.766 | 1.00 31.45 | TAW |
| ATOM | 1016 | o | HOH | 92 | | 11.773 | 44.998 | 1.00 29.99 | WAT |
| MOTA | 1017 | o | нон | 93 | -1.506 -3.463 | 7.951 | 67.587 | 1.00 28.61 | TAW |
| ATOM | 1018 | 0 | НОН | 93 94 | -3.462 -2.310 | 10.383 | 67.429 | 1.00 32.97 | WAT |
| ATOM | 1019 | o | нон | 95 | | 12.680 | 66.265 | 1.00 27.88 | WAT |
| ATOM | 1020 | o | нон | 96 | -4.299 | 16.505 | 66.744 | 1.00 34.32 | WAT |
| MOTA | 1021 | Ö | нон | 9 7 | 0.990 | 24.911 | | 1.00 31.02 | WAT |
| ATOM | 1022 | ŏ | нон | 98 | -13.635 | 13.854 | 63.282 | 1.00 15.69 | WAT |
| ATOM | 1022 | Ö | нон | | -12.472 | 13.178 | 48.835 | 1.00 25.84 | WAT |
| ATOM | 1023 | N1 | | 99 | 0.796 | 0.192 | 42.865 | 1.00 28.22 | WAT |
| | | | COA | 120 | -12.948 | 7.608 | 44.920 | 1.00 13.13 | COA |
| ATOM | 1025 | C2 | COA | 120 | -11.643 | 7.336 | 45.414 | 1.00 12.29 | COA |
| ATOM | 1026 | ИЗ | COA | 120 | -11.182 | 7.731 | 46.667 | 1.00 13.13 | COA |
| MOTA | 1027 | C4 | COA | 120 | -12.090 | 8.415 | 47.420 | 1.00 12.87 | COA |
| ATOM | 1028 | C5 | COA | 120 | -13.461 | 8.771 | 47.064 | 1.00 12.68 | COA |
| ATOM | 1029 | C6 | COA | 120 | -13.899 | 8.321 | 45.698 | 1.00 13.32 | COA |
| ATOM | 1030 | N6 | COA | 120 | -15.094 | 8.573 | 45.246 | 1.00 13.97 | COA |
| MOTA | 1031 | N7 | COA | 120 | -14.087 | 9.450 | 48.042 | 1.00 13.45 | COA |
| MOTA | 1032 | C8 | COA | 120 | -13.179 | 9.555 | 49.021 | 1.00 14.05 | COA |
| MOTA | 1033 | И9 | COA | 120 | -11.940 | 8.949 | 48.707 | 1.00 12.82 | COA . |
| ATOM | 1034 | | COA | 120 | -10.508 | 8.739 | 49.433 | 1.00 12.92 | COA |
| MOTA | 1035 | C2* | COA | 120 | -10.131 | 10.063 | 49.988 | 1.00 12.61 | COA |
| | | | | | | | | | 3 |

| MOTA | 409 | CD2 | LEU | 50 | -0.213 | 19.390 | 58.824 | 1.00 13.78 | ACPS |
|--------------|------------|----------|------------|----------|------------------|------------------|------------------|------------------------|--------------|
| MOTA | 410 | C | LEU | 50 | -1.573 | 15.900 | 56.413 | 1.00 10.56 | ACPS |
| MOTA | 411 | 0 | LEU | 50 | -0.684 | 15.827 | 55.569 | 1.00 10.55 | ACPS |
| MOTA | 412 | N | ALA | 51 | -1.806 | 14.936 | 57.301 | 1.00 10.65 | ACPS |
| ATOM | 413 | CA | ALA | 51 | -1.001 | 13.711 | 57.291 | 1.00 10.86 | ACPS |
| MOTA | 414 | CB | ALA | 51 | -1.330 | 12.847 | 58.510 | 1.00 10.65 | ACPS |
| MOTA | 415 | С | ALA | 51 | -1.213 | 12.905 | 56.003 | 1.00 11.03 | ACPS |
| MOTA | 416 | 0 | ALA | 51 | -0.274 | 12.296 | 55.481 | 1.00 10.16 | ACPS |
| MOTA | 417 | N | GLY | 52 | -2.441 | 12.913 | 55.490 | 1.00 11.30 | ACPS |
| MOTA | 418 | CA | GLY | 52 | -2.742 | 12.186 | 54.267 | 1.00 11.27 | ACPS |
| MOTA | 419 | C | GLY | 52 | -2.113 | 12.848 | 53.050 | 1.00 11.12 | ACPS |
| MOTA | 420 | 0 | GLY | 52 | -1.635 | 12.174 | 52.144 | 1.00 10.32 | ACPS |
| MOTA | 421 | N | ARG | 53 | -2.118 | 14.177 | 53.026 | 1.00 10.73 | ACPS ACPS |
| ATOM | 422 | CA | ARG | 53 53 | -1.521 | 14.896 | 51.906 51.943 | 1.00 10.83 | ACPS |
| MOTA | 423 | CB | ARG | 53 53 | -1.919 -3.089 | 16.385 16.756 | 51.012 | 1.00 11.05 | ACPS |
| ATOM | 424 | CG | ARG ARG | 53 | -4.316 | 15.894 | 51.232 | 1.00 14.65 | ACPS |
| MOTA MOTA | 425 426 | CD NE | ARG | 53 | -5.419 | 16.229 | 50.322 | 1.00 13.75 | ACPS |
| ATOM | 427 | CZ | ARG | 53 | -6.569 | 15.562 | 50.280 | 1.00 14.79 | ACPS |
| ATOM | 428 | | ARG | 53 | -6.761 | 14.525 | 51.087 | 1.00 14.78 | ACPS |
| ATOM | 429 | | ARG | 53 | -7.534 | 15.932 | 49.445 | 1.00 15.39 | ACPS |
| ATOM | 430 | C | ARG | 53 | 0.001 | 14.732 | 51.974 | 1.00 10.44 | ACPS |
| ATOM | 431 | ō | ARG | 53 | 0.654 | 14.603 | 50.938 | 1.00 10.68 | ACPS |
| ATOM | 432 | N | PHE | 54 | 0.557 | 14.728 | 53.193 | 1.00 10.64 | ACPS |
| ATOM | 433 | CA | PHE | 54 | 1.999 | 14.549 | 53.396 | 1.00 9.72 | ACPS |
| ATOM | 434 | CB | PHE | 54 | 2.308 | 14.710 | 54.903 | 1.00 10.85 | ACPS |
| MOTA | 435 | CG | PHE | 54 | 3.770 | 14.621 | 55.264 | 1.00 11.55 | ACPS |
| MOTA | 436 | CD1 | PHE | 54 | 4.397 | 13.386 | 55.407 | 1.00 12.45 | ACPS |
| MOTA | 437 | CD2 | PHE | 54 | 4.505 | 15.780 | 55.522 | 1.00 12.56 | ACPS |
| ATOM | 438 | CE1 | PHE | 54 | 5.729 | 13.301 | 55.806 | 1.00 12.31 | ACPS |
| MOTA | 439 | | PHE | 54 | 5.841 | 15.709 | 55.923 | 1.00 11.84 | ACPS |
| ATOM | 440 | CZ | PHE | 54 | 6.452 | 14.462 | 56.066 | 1.00 13.57 | ACPS |
| ATOM | 441 | C | PHE | 54 | 2.392 | 13.154 | 52.861 | 1.00 9.79 | ACPS |
| ATOM | 442 | 0 | PHE | 54 | 3.377 | 13.010 | 52.123 | 1.00 9.57 | ACPS |
| MOTA | 443 | N | ALA | 55 55 | 1.607 | 12.136 | 53.210 | 1.00 9.67 | ACPS |
| ATOM | 444 | CA | ALA | 55 55 | 1.873 | 10.770 | 52.742 | 1.00 9.05 1.00 9.23 | ACPS ACPS |
| ATOM | 445 | СВ | ALA | 55 55 | 0.894 | 9.788 10.694 | 53.396 51.218 | 1.00 9.72 | ACPS |
| MOTA | 446 | C | ALA ALA | 55 55 | 1.758 2.578 | 10.070 | 50.550 | 1.00 10.39 | ACPS |
| MOTA | 447 448 | o N | ALA | 56 | 0.730 | 11.327 | 50.666 | 1.00 10.39 | ACPS |
| ATOM ATOM | 449 | CA | ALA | 56 | 0.750 | 11.313 | 49.215 | 1.00 9.78 | ACPS |
| ATOM | 450 | CB | ALA | 56 | -0.759 | 12.014 | 48.846 | | ACPS |
| ATOM | 451 | C | ALA | 56 | 1.728 | 11.969 | 48.487 | 1.00 9.83 | ACPS |
| ATOM | 452 | o | ALA | 56 | 2.158 | 11.479 | 47.451 | 1.00 10.05 | ACPS |
| ATOM | 453 | N | LYS | 57 | 2.242 | 13.077 | 49.026 | 1.00 9.72 | ACPS |
| ATOM | 454 | CA | LYS | 57 | 3.361 | 13.758 | 48.388 | 1.00 10.49 | ACPS |
| ATOM | 455 | CB | LYS | 57 | 3.477 | 15.194 | 48.914 | 1.00 9.29 | ACPS |
| ATOM | 456 | CG | LYS | 57 | 2.243 | 16.015 | 48.546 | 1.00 9.85 | ACPS |
| ATOM | 457 | CD | LYS | 57 | 2.383 | 17.492 | 48.881 | 1.00 10.42 | ACPS |
| ATOM | 458 | CE | LYS | 57 | 1.057 | 18.196 | 48.628 | 1.00 10.41 | ACPS |
| ATOM | 459 | NZ | LYS | 57 | 1.214 | 19.689 | 48.629 | 1.00 10.56 | ACPS |
| ATOM | 460 | C | LYS | 57 | 4.668 | 12.986 | 48.549 | 1.00 10.05 | ACPS |
| ATOM | 461 | ō | LYS | 57 | 5.501 | 12.992 | 47.632 | 1.00 11.38 | ACPS |
| ATOM | 462 | N | GLU | 58 | 4.863 | 12.322 | 49.687 | 1.00 10.76 | ACPS |
| ATOM | 463 | CA | GLU | 58 | 6.073 | 11.513 | 49.846 | 1.00 10.03 | ACPS |
| ATOM | 464 | CB | GLU | 58 | 6.270 | 11.064 | 51.304 | 1.00 10.79 | ACPS |
| ATOM | 465 | CG | GLU | 58 | 6.674 | 12.221 | 52.234 | 1.00 12.67 | ACPS |
| | | | | | | | | | |

| ATOM | 1036 | 5 021 | COA | 120 | -8.885 | 10.585 | 49.617 | 1.00 13.09 | COA |
|------|------|-------|-----|-----|---------|--------|--------|------------|------|
| ATOM | 1037 | | | | -10.321 | 9.967 | 51.470 | 1.00 12.95 | COA |
| ATOM | 1038 | 3 03* | | | -9.269 | 10.478 | 52.488 | 1.00 12.93 | COA |
| ATOM | 1039 | P3* | COA | | -9.182 | 12.127 | 52.589 | 1.00 13.47 | COA |
| ATOM | 1040 | 07 | COA | | -8.835 | 12.768 | 51.184 | 1.00 13.51 | COA |
| ATOM | 1041 | . 08 | COA | | -8.049 | 12.448 | 53.626 | 1.00 13.28 | COA |
| ATOM | 1042 | | COA | | -10.609 | 12.596 | 53.131 | 1.00 14.44 | COA |
| ATOM | 1043 | | | 120 | -10.208 | 8.375 | 51.725 | 1.00 13.08 | COA |
| ATOM | 1044 | | COA | 120 | -10.977 | 7.897 | 50.509 | 1.00 12.26 | COA |
| ATOM | 1045 | | COA | 120 | -10.401 | 7.949 | 53.127 | 1.00 14.58 | COA |
| ATOM | 1046 | 05* | COA | 120 | -10.469 | 6.473 | 52.938 | 1.00 13.48 | COA |
| ATOM | 1047 | P1 | COA | 120 | -10.652 | 5.672 | 54.364 | 1.00 12.56 | COA |
| ATOM | 1048 | 01 | COA | 120 | -9.729 | 6.240 | 55.365 | 1.00 13.21 | COA |
| MOTA | 1049 | 02 | COA | 120 | -10.459 | 4.226 | 54.119 | 1.00 15.04 | COA |
| MOTA | 1050 | 03 | COA | 120 | -12.029 | 6.083 | 54.854 | 1.00 16.52 | COA |
| ATOM | 1051 | . P2 | COA | 120 | -13.553 | 5.541 | 54.845 | 1.00 22.65 | COA |
| ATOM | 1052 | 04 | COA | 120 | -13.663 | 4.249 | 55.488 | 1.00 23.91 | COA |
| MOTA | 1053 | 05 | COA | 120 | -14.429 | 6.530 | 55.551 | 1.00 25.17 | COA |
| ATOM | 1054 | 06 | COA | 120 | -13.926 | 5.591 | 53.277 | 1.00 23.32 | COA |
| MCTA | 1055 | C11 | COA | 120 | -14.755 | 4.650 | 51.149 | 1.00 25.32 | COA |
| MOTA | 1056 | | COA | 120 | -13.824 | 4.473 | 52.426 | 1.00 24.46 | COA |
| MOTA | 1057 | C13 | COA | 120 | -14.105 | 5.689 | 50.154 | 1.00 25.05 | COA |
| ATOM | 1058 | C14 | COA | 120 | -14.799 | 3.243 | 50.564 | 1.00 25.09 | COA |
| ATOM | 1059 | | COA | 120 | -16.252 | 5.244 | 51.556 | 1.00 26.37 | COA |
| ATOM | 1060 | | COA | 120 | -17.086 | 5.395 | 50.361 | 1.00 26.75 | COA |
| MOTA | 1061 | C9 | COA | 120 | -17.067 | 4.353 | 52.553 | 1.00 27.72 | COA |
| MOTA | 1062 | | COA | 120 | -16.649 | 4.199 | 53.819 | 1.00 28.04 | COA |
| ATOM | 1063 | И8 | COA | 120 | -18.144 | 3.780 | 52.101 | 1.00 30.34 | COA |
| ATOM | 1064 | C7 | COA | 120 | -19.329 | 3.490 | 52.916 | 1.00 32.23 | COA |
| ATOM | 1065 | C42 | | 120 | -19.224 | 2.064 | 53.477 | | COA |
| ATOM | 1066 | | COA | 120 | -19.805 | 1.971 | 54.888 | 1.00 34.86 | COA |
| ATOM | 1067 | | COA | 120 | -20.414 | 2.967 | 55.487 | 1.00 36.24 | COA |
| ATOM | 1068 | N4 | COA | 120 | -19.632 | 0.789 | 55.446 | 1.00 34.84 | COA |
| ATOM | 1069 | C3 | COA | 120 | -20.112 | 0.432 | 56.852 | 1.00 34.67 | COA |
| ATOM | 1070 | | COA | 120 | -19.736 | -0.998 | 57.112 | 1.00 34.47 | COA |
| ATOM | 1071 | S1 | COA | 120 | -20.877 | -2.208 | 56.301 | 1.00 33.46 | COA |
| ATOM | | CA+2 | | 1 | 7.365 | 8.523 | 54.928 | 1.00 11.64 | IONS |
| ATOM | | CL-1 | | 2 | 5.841 | 9.868 | 59.601 | 1.00 16.02 | IONS |
| ATOM | 1074 | CA+2 | CA2 | 3 | 0.000 | 0.000 | 65.920 | 0.33 1.00 | IONS |
| END | | | | | | | | | |



Figure 3A





Figure 3B

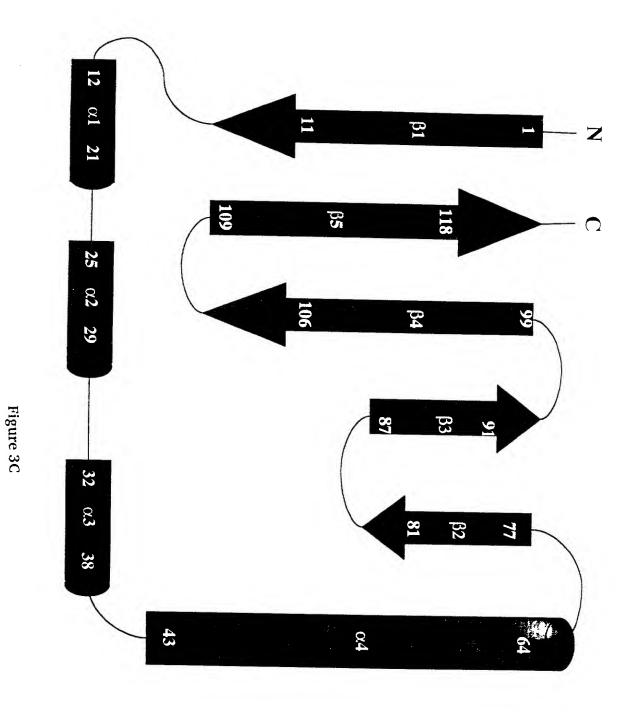




Figure 4



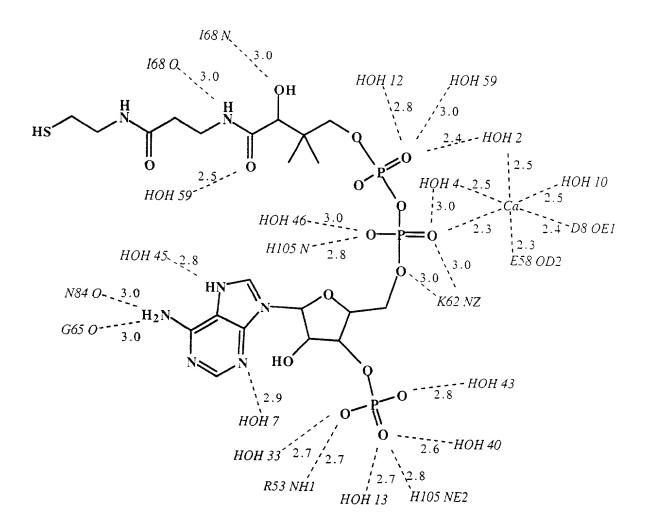


Figure 5

Figure 6

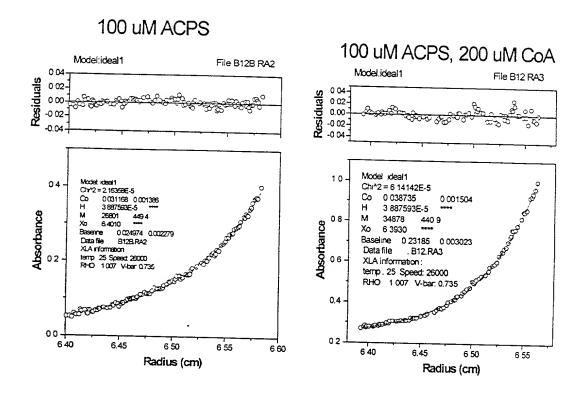
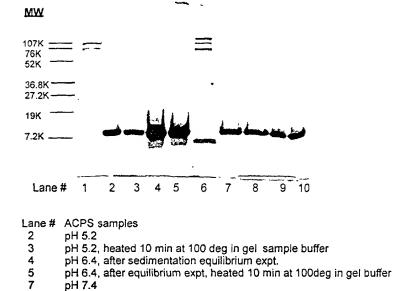


Figure 7

15% Non-reducing, denaturing gel of ACPS samples before and after analytical centrifugation



Lanes 2, 3, 7, 8, 9, 10: 20 uL of a freshly prepared 32 uJM ACPS sample was added Lanes 4, 5: 20 uL of the 100 uM ACPS pH 6.4 solution from the sedimentation equilibrium experiment was used

pH 6.4, heated 10 min at 100 deg in gel sample buffer

pH 7.4, heated 10 min at 100 deg in gel buffer

8

9

10

pH 6.4

| MIYGI | GLDIT | ELKRI | ASMAG | RQKRF | AERIL |
|-------|-------|-------|-------|-------|-------|
| TRSEL | DQYYE | LSEKR | KNEFL | AGRFA | AKEAF |
| SKAFG | TGIGR | QLSFQ | DIEIR | KDQNG | KPYII |
| CTKLS | QAAVH | VSITH | TKEYA | AAQVV | IERLS |
| S | | | | | |

Figure 8

